Exploiting Mixed Precision in Numerical Linear Algebra

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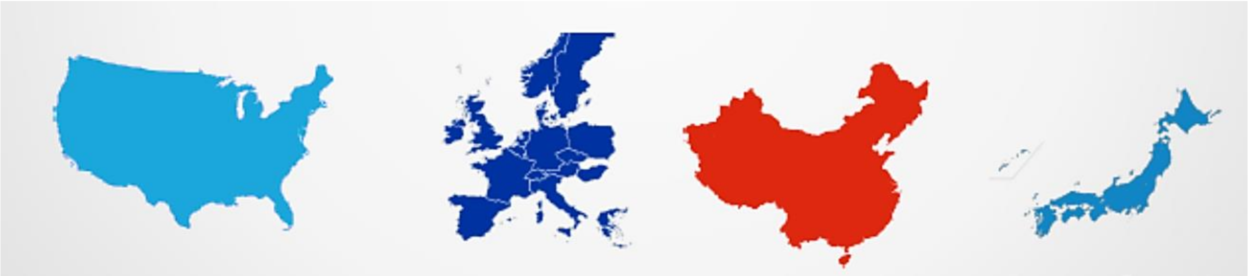
Exascale Computing: A Modern Space Race

- "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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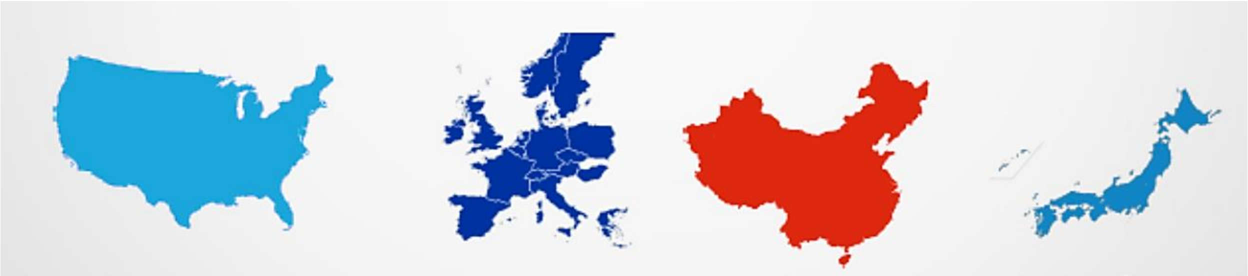

- Technical challenges at all levels

hardware to algorithms to applications

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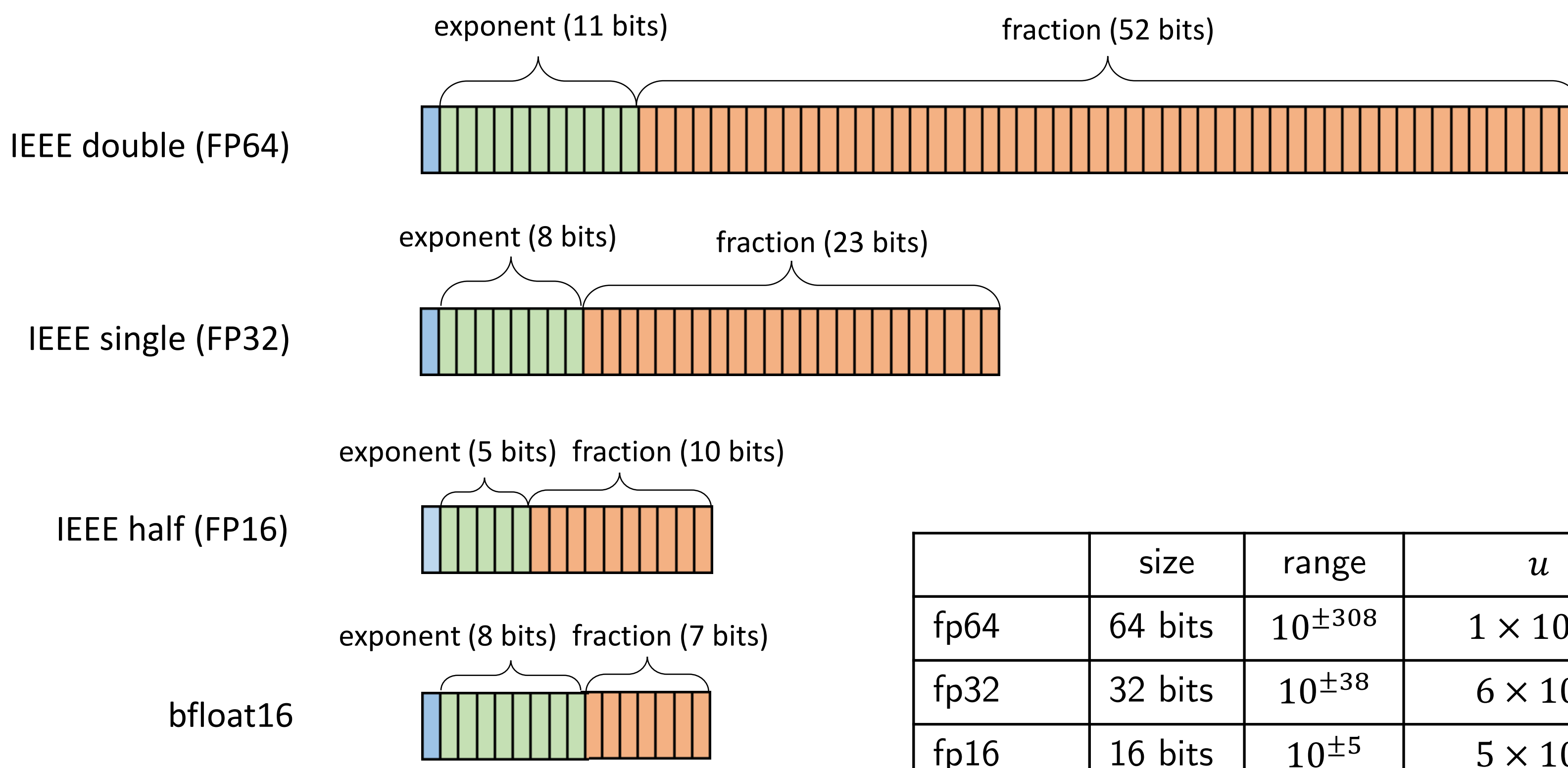
Floating Point Formats

$$(-1)^{\text{sign}} \times 2^{(\text{exponent}-\text{offset})} \times 1.\text{fraction}$$



	size	range	u
fp64	64 bits	$10^{\pm 308}$	1×10^{-16}
fp32	32 bits	$10^{\pm 38}$	6×10^{-8}
fp16	16 bits	$10^{\pm 5}$	5×10^{-4}
bfloat16	16 bits	$10^{\pm 38}$	4×10^{-3}

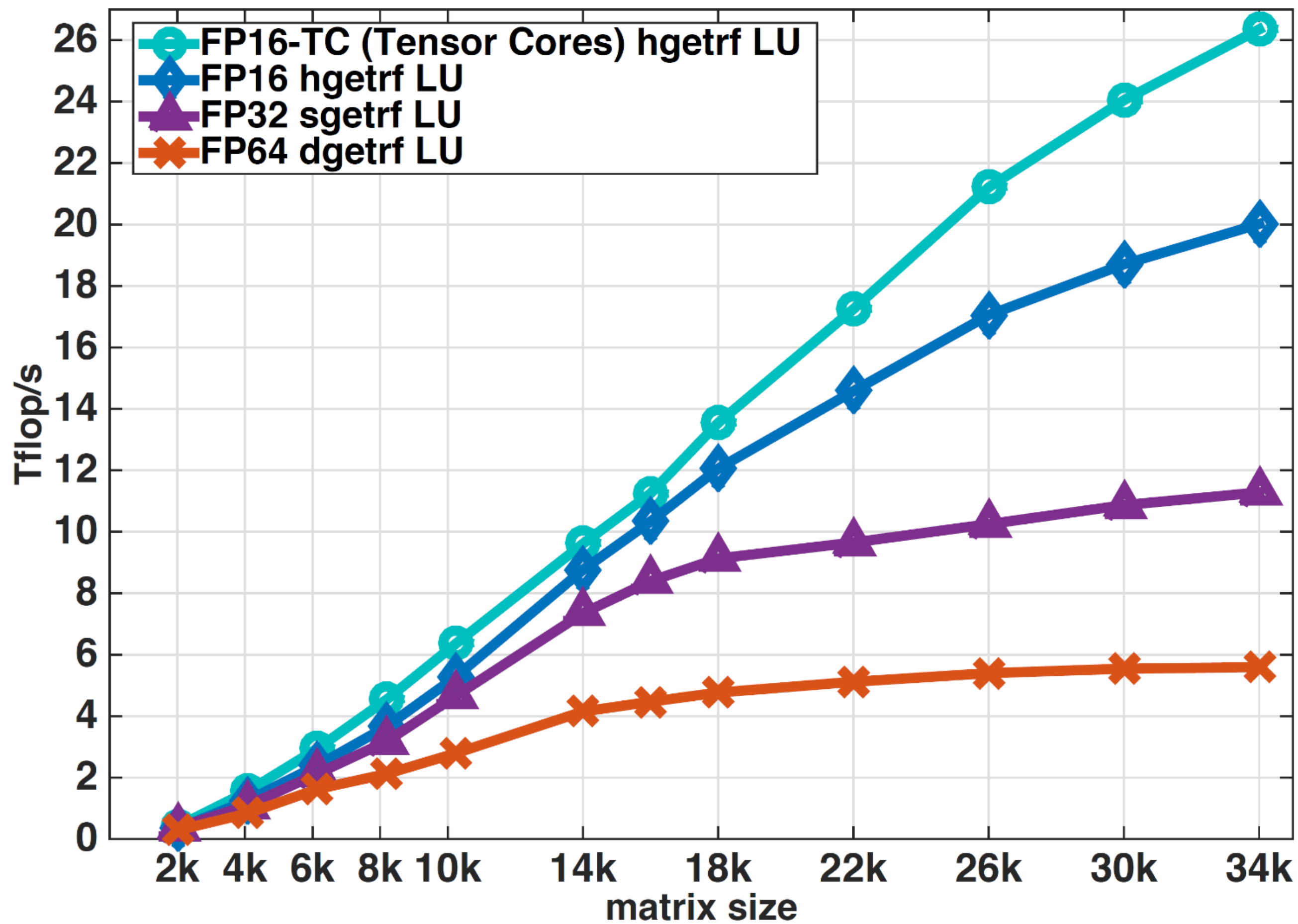
Hardware Support for Multiprecision Computation

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!**)
- NVIDIA A100, 2020: tensor cores with multiple supported precisions: FP16, FP64, Binary, INT4, INT8, bfloat16
- Google's Tensor processing unit (TPU)
- 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]

Mixed Precision Capabilities on Supercomputers

From TOP500:

June 2021

	Accelerator/CP Family	Count	System Share (%)	Rmax (GFlops)	Rpeak (GFlops)	Cores
1	NVIDIA Volta	97	19.4	626,503,420	1,049,977,600	11,875,056
2	NVIDIA Ampere	26	5.2	351,252,600	505,841,268	3,435,116
3	NVIDIA Pascal	9	1.8	57,876,640	85,807,525	1,141,300

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June 2019

	Accelerator/CP Family	Count	System Share (%)	Rmax (GFlops)	Rpeak (GFlops)	Cores
1	NVIDIA Pascal	61	12.2	106,025,166	179,951,012	2,738,356
3	NVIDIA Volta	12	2.4	224,559,400	360,593,742	4,488,720

An exaflop of what?

- When will victory be declared?
  - When a supercomputer reaches exaflop performance on the HPL (LINPACK) benchmark (TOP500)
    - Solving dense $Ax = b$ using Gaussian elimination with partial pivoting in double precision (FP64)

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- HPL benchmark is typically a compute-bound problem ("BLAS-3")
- Not a good indication of performance for a large number of applications!
  - Lots of remaining work even after exascale performance is achieved
  - Has led to incorporation of other benchmarks into the TOP500 ranking
    - e.g., HPCG: Solving sparse $Ax = b$ iteratively using the conjugate gradient method

An exaflop of what?

- HPL doesn't make use of modern mixed precision hardware

- We can *already* achieve "exaflop" performance today if we allow for mixed precision computations

https://www.olcf.ornl.gov/2018/06/08/genomics-code-exceeds-exaops-on-summit-supercomputer/

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=>HPL-AI: A new mixed precision benchmark

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)

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

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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"Fixed-Precision"

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

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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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Iterative Refinement in 3 Precisions

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$\Rightarrow$ **3-precision iterative refinement**

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

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

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

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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 Aspects of Analysis 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

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

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

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$$\boldsymbol{u_s}\|E_i\|_\infty \leq 3n\boldsymbol{u_f}\left\||A^{-1}||\hat{L}||\hat{U}|\right\|_\infty$$

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

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$u_s\|E_i\|_\infty \leq 3nu_f\left\||A^{-1}||\hat{L}||\hat{U}|\right\|_\infty$

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3. $\left| \hat{r}_i - A\hat{d}_i \right| \le u_s G_i |\hat{d}_i|$

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E_i, c_1, c_2, and G_i depend on A, $\hat{r}_i$, n, and 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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$$\phi_i \equiv (c_1 \kappa_\infty(A) + c_2)\boldsymbol{u_s}$$

is 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}
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}	$\mathrm{cond}(A,x) \cdot 10^{-8}$
	H	S	D	10^4	10^{-8}	10^{-8}	10^{-8}
LP fact.	H	D	D	10^4	10^{-16}	10^{-16}	$\mathrm{cond}(A,x) \cdot 10^{-16}$
	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}
LP fact.	S	D	D	10^8	10^{-16}	10^{-16}	$\mathrm{cond}(A,x) \cdot 10^{-16}$
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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}
Fixed	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	S	D	10^4	10^{-8}	10^{-8}	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}	$\text{cond}(A,x) \cdot 10^{-8}$
Trad.	S	S	D	10^8	10^{-8}	10^{-8}	10^{-8}
LP fact.	S	D	D	10^8	10^{-16}	10^{-16}	$\text{cond}(A,x) \cdot 10^{-16}$
	S	D	Q	10^8	10^{-16}	10^{-16}	10^{-16}

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

IR3: Summary

Standard (LU-based) IR in three precisions ($u_s = u_f$)

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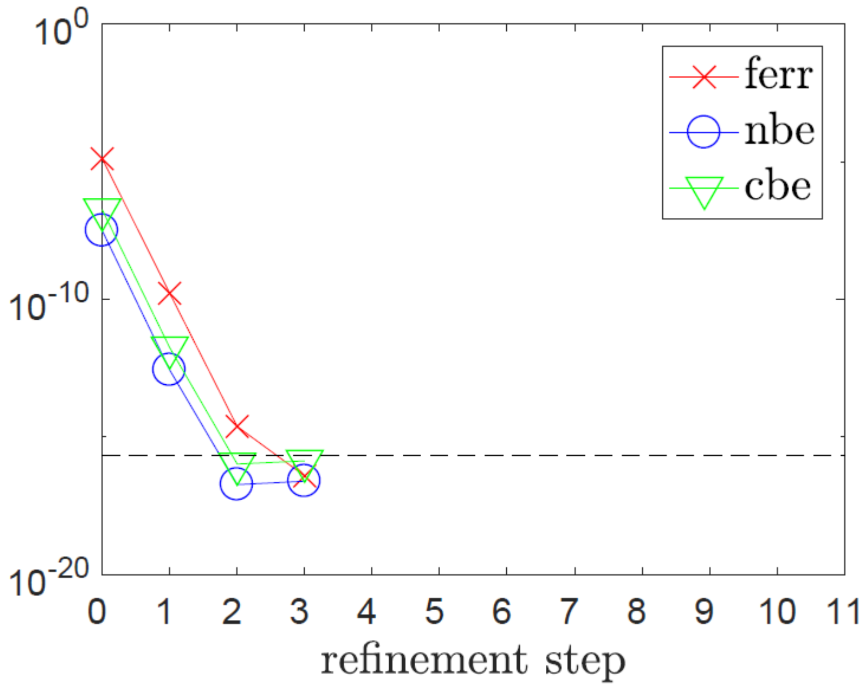
New	S	D	Q	10^8	10^{-16}	10^{-16}	10^{-16}

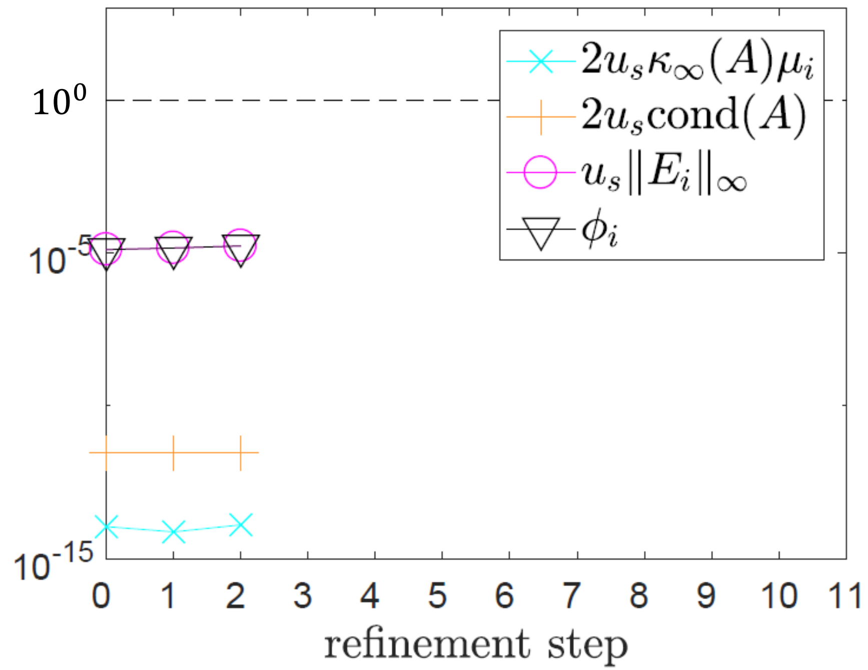
$\Rightarrow$ Benefit of IR3 vs. traditional IR: As long as $\kappa_\infty(A) \leq 10^4$, can use lower precision factorization w/no loss of accuracy!

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

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

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

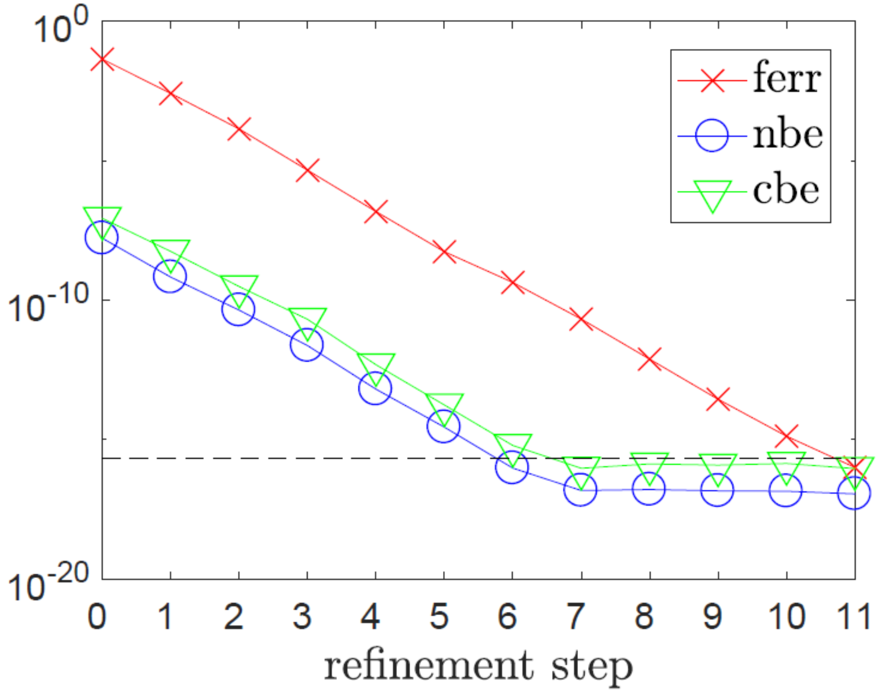


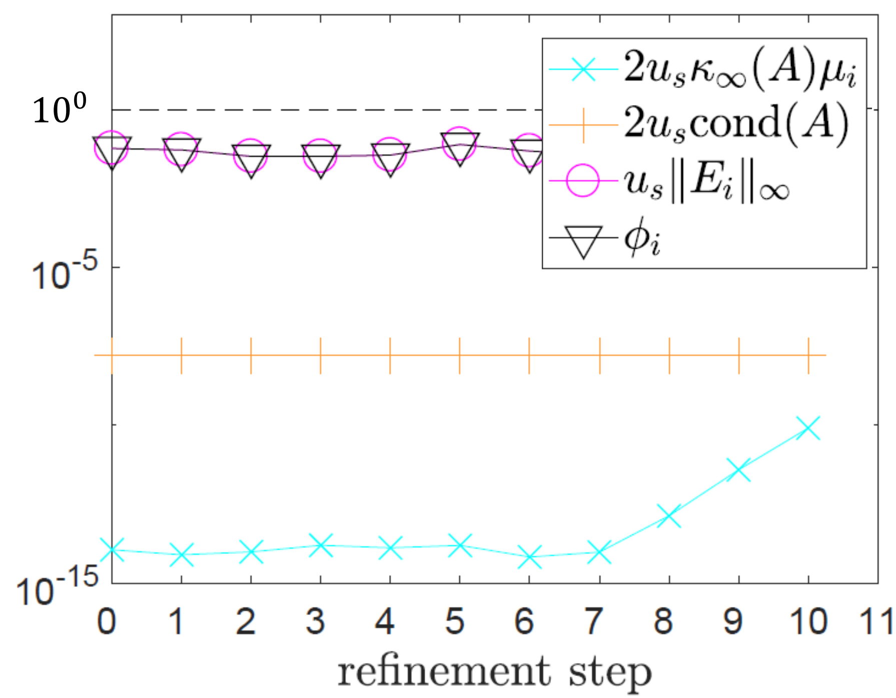


```
A = gallery('randsvd', 100, 1e7)
b = randn(100,1)
```

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

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

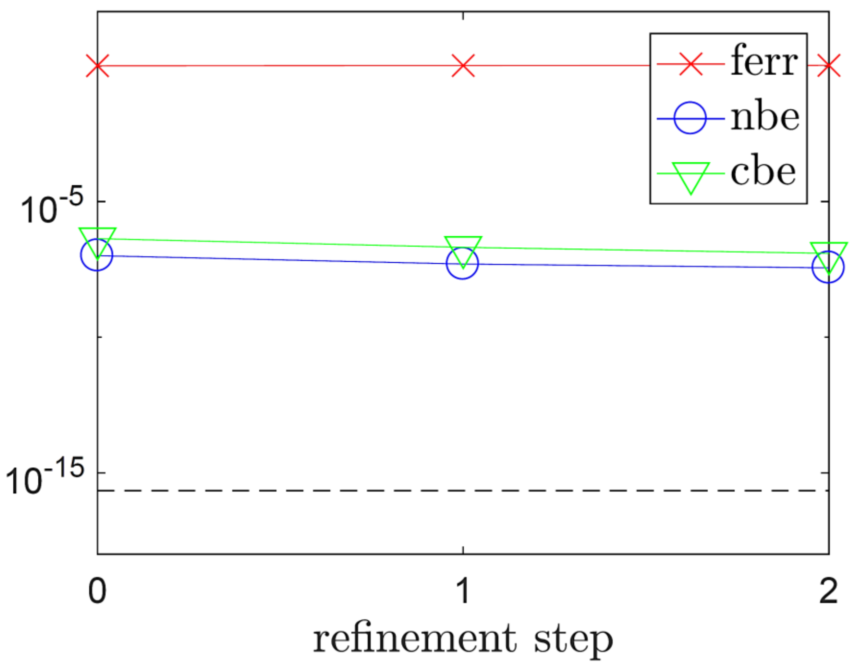


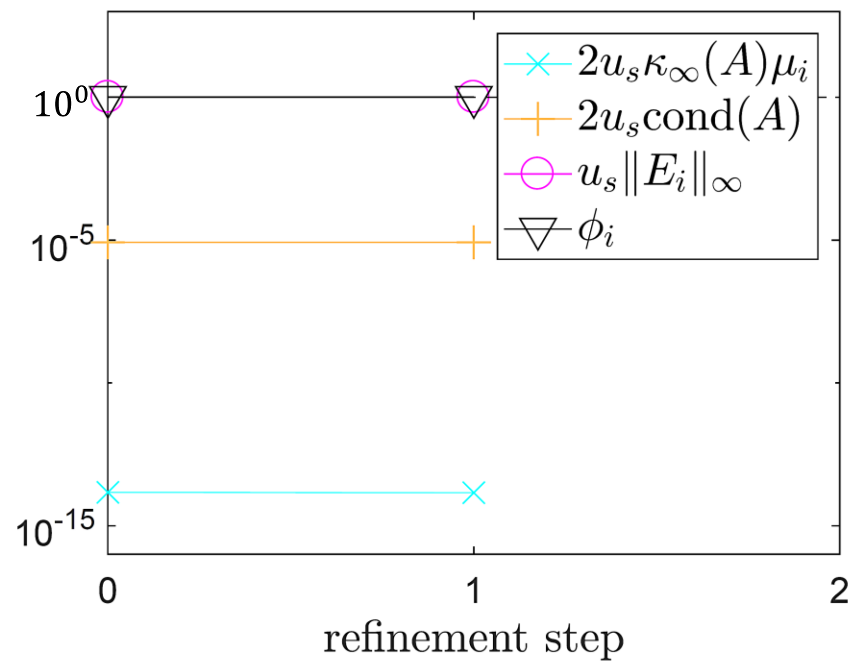


```
A = gallery('randsvd', 100, 1e9)
b = randn(100,1)
```

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

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





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```

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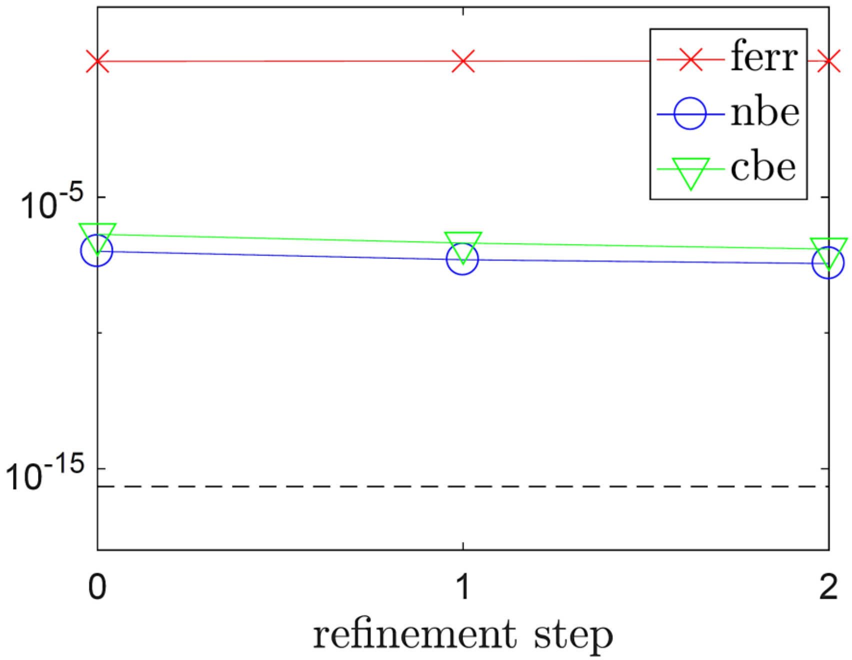
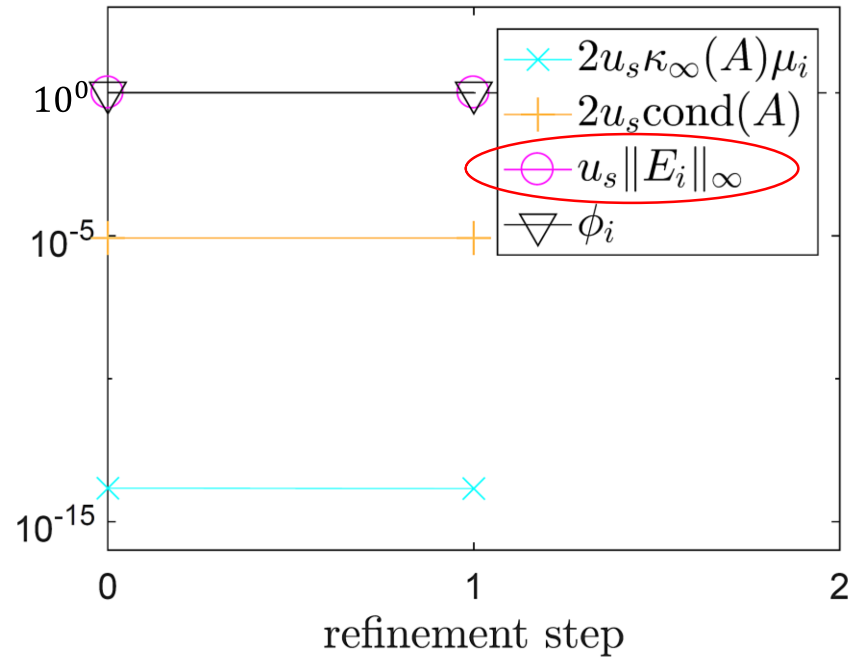
Standard (LU-based) IR with u_f: single, u: double, u_r: quad

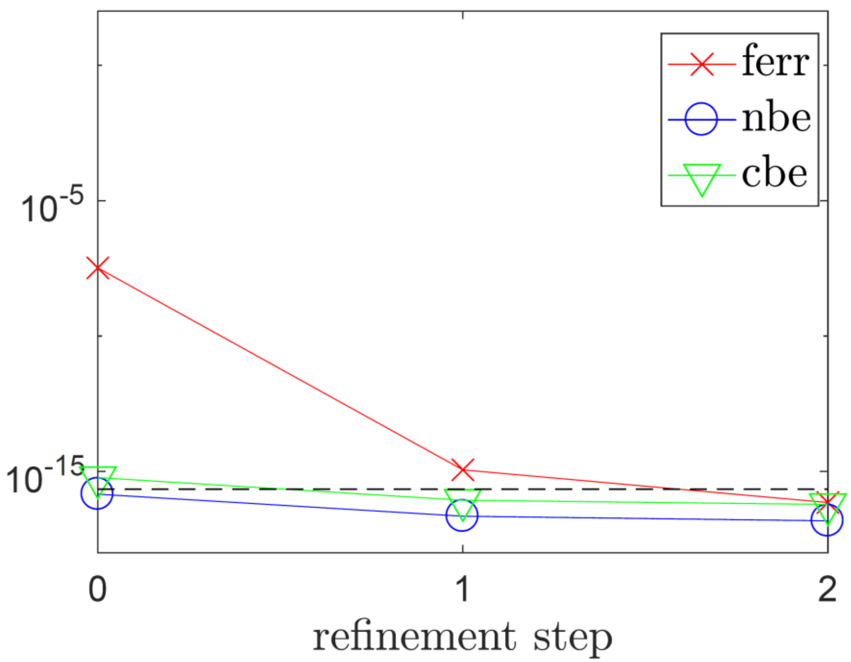


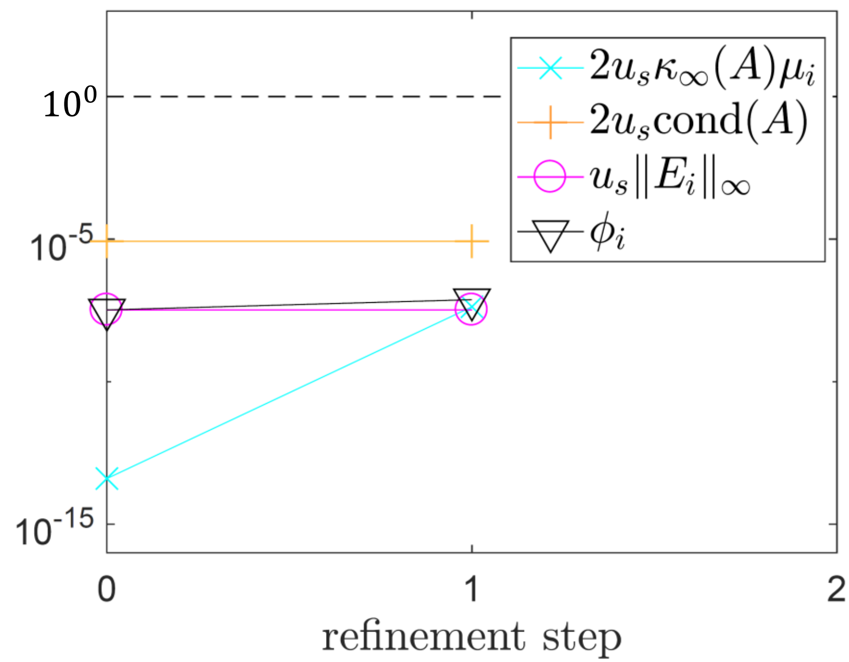


```
A = gallery('randsvd', 100, 1e9)
b = randn(100,1)
```

$\boldsymbol{\kappa_\infty(A)} \approx$ **2e10**

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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<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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Solve $Ax_0 = b$ by LU factorization

for $i = 0$: maxit

$r_i = b - Ax_i$

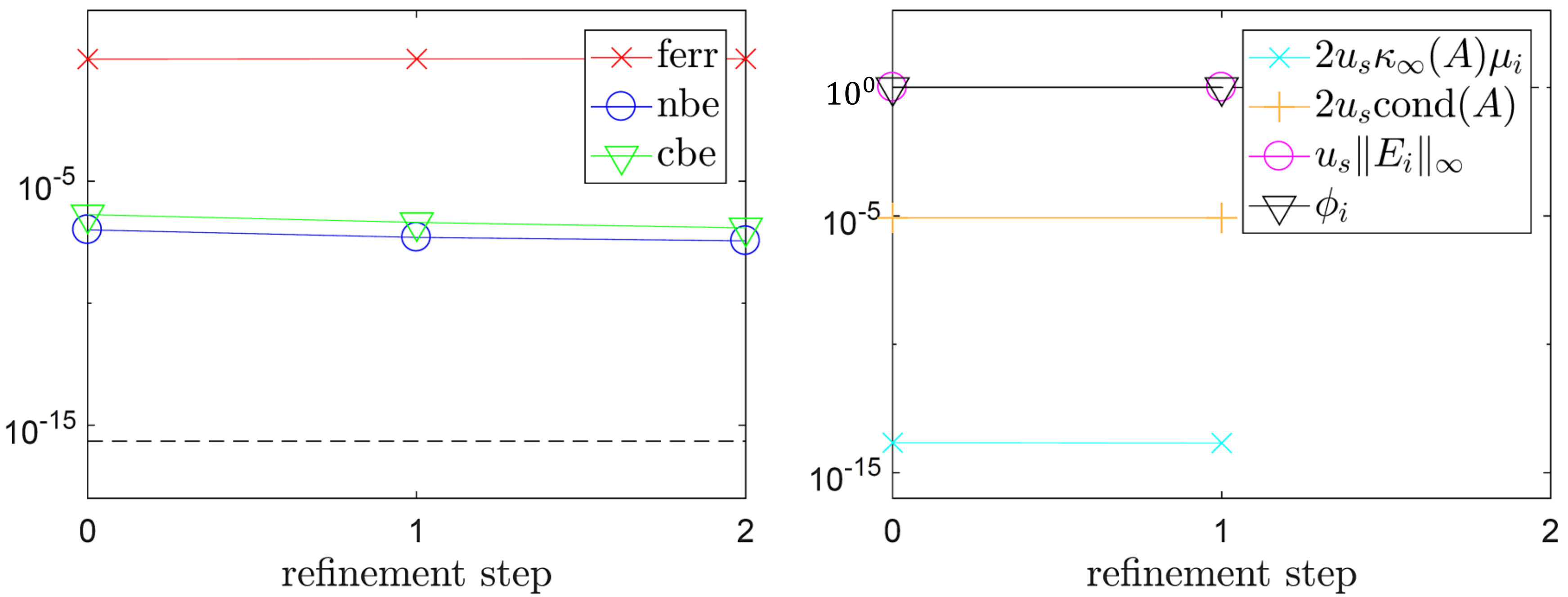
Solve $Ad_i = r_i$ via GMRES on $\tilde{A}d_i = \tilde{r}_i$ → $\boldsymbol{u_s} = \boldsymbol{u}$

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

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

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

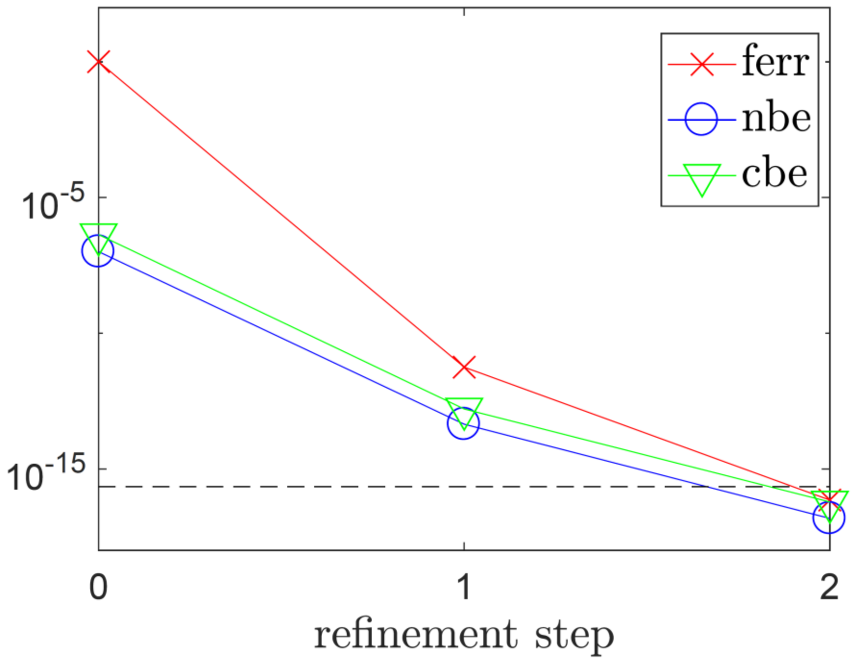
Standard (LU-based) IR with u_f: single, u: double, u_r: quad

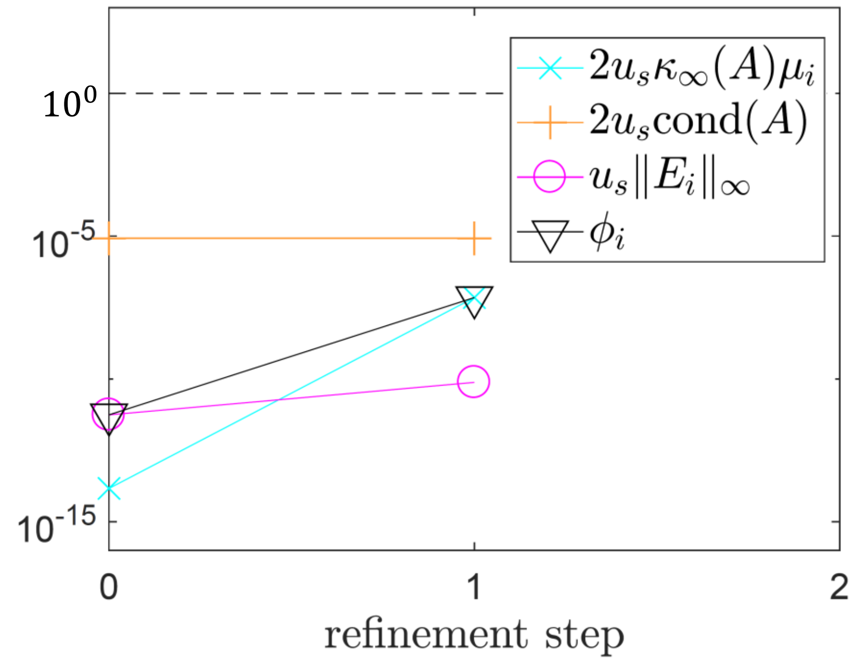


```
A = gallery('randsvd', 100, 1e9, 2)
b = randn(100,1)
```

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

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





Number of GMRES iterations: (2,3)

GMRES-IR: Summary

Benefits of GMRES-IR:

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

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

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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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}

⇒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

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}
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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}

$\Rightarrow$ As long as $\kappa_\infty(A) \leq 10^{12}$, can use half precision factorization and still obtain double precision accuracy!

Comments and Caveats I

- Convergence tolerance τ for GMRES?
  - Smaller $\tau \rightarrow$ more GMRES iterations, potentially fewer refinement steps
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- What about overflow, underflow, subnormal numbers?
  - Sophisticated scaling methods can help avoid this
    - "Squeezing a Matrix into Half Precision, with an Application to Solving Linear Systems" [Higham, Pranesh, Zounon, 2019]

Comments and Caveats II

- Convergence rate of GMRES?

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  - If A is ill conditioned and LU factorization is performed in very low precision, it can be a poor preconditioner
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- Depending on conditioning of A, applying $\tilde{A}$ to a vector must be done accurately (precision u^2) in each GMRES iteration
  - Recent development of 5-precision GMRES-IR algorithm [Amestoy et al., 2021]
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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!

GMRES-IR in Libraries and Applications

- MAGMA: Dense linear algebra routines for heterogeneous/hybrid architectures

magma / src / dxgesv_gmres_gpu.cpp

```
-------
DSGESV or DHGESV expert interface.
It computes the solution to a real system of linear equations
   A * X = B,  A**T * X = B,  or  A**H * X = B,
where A is an N-by-N matrix and X and B are N-by-NRHS matrices.
the accomodate the Single Precision DSGESV and the Half precision dhgesv API.
precision and iterative refinement solver are specified by facto_type, solver_type.
For other API parameter please refer to the corresponding dsgesv or dhgesv.
```

- NVIDIA's cuSOLVER Library

2.2.1.6. cusolverIRSRefinement_t

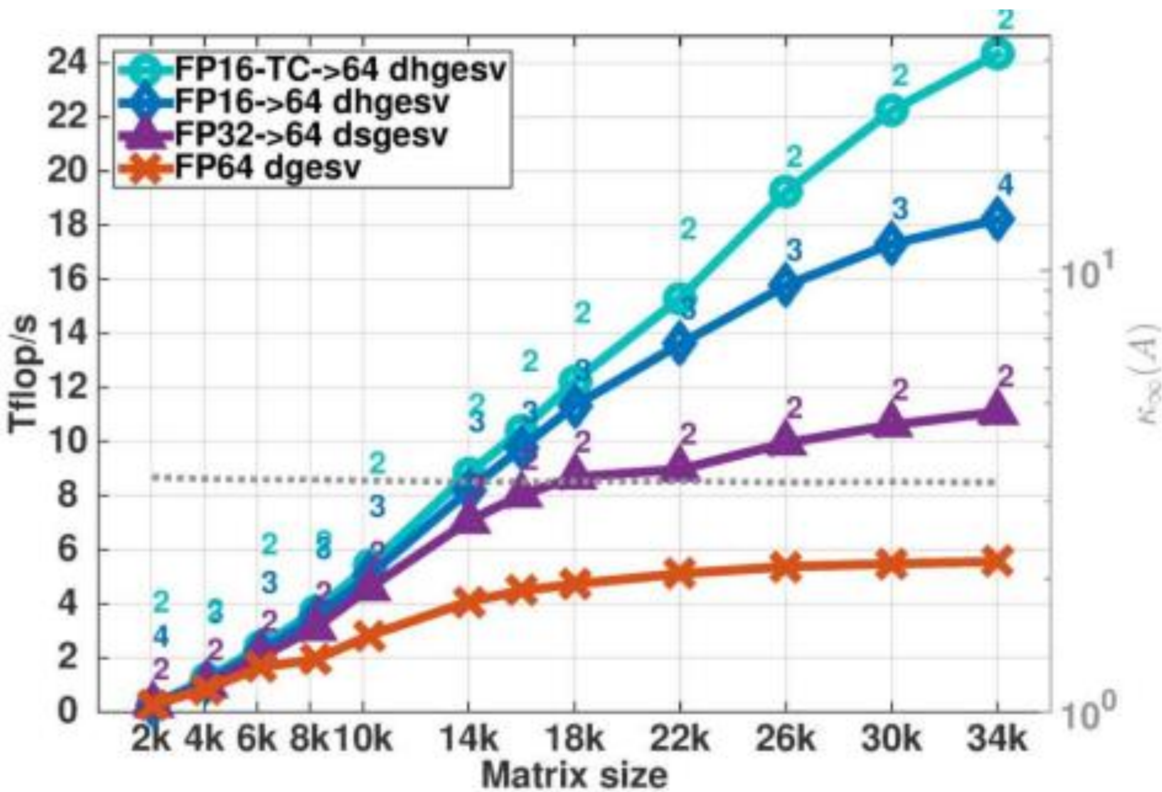
The `cusolverIRSRefinement_t` type indicates which solver type would be used for the specific cusolver function. Most of our experimentation shows that CUSOLVER_IRS_REFINE_GMRES is the best option.

`CUSOLVER_IRS_REFINE_GMRES`	GMRES (Generalized Minimal Residual) based iterative refinement solver. In recent study, the GMRES method has drawn the scientific community attention for its ability to be used as refinement solver that outperforms the classical iterative refinement method. based on our experimentation, we recommend this setting.

- In production codes: FK6D/ASGarD code (Oak Ridge National Lab, USA) for tokomak containment problem

Performance Results (MAGMA)

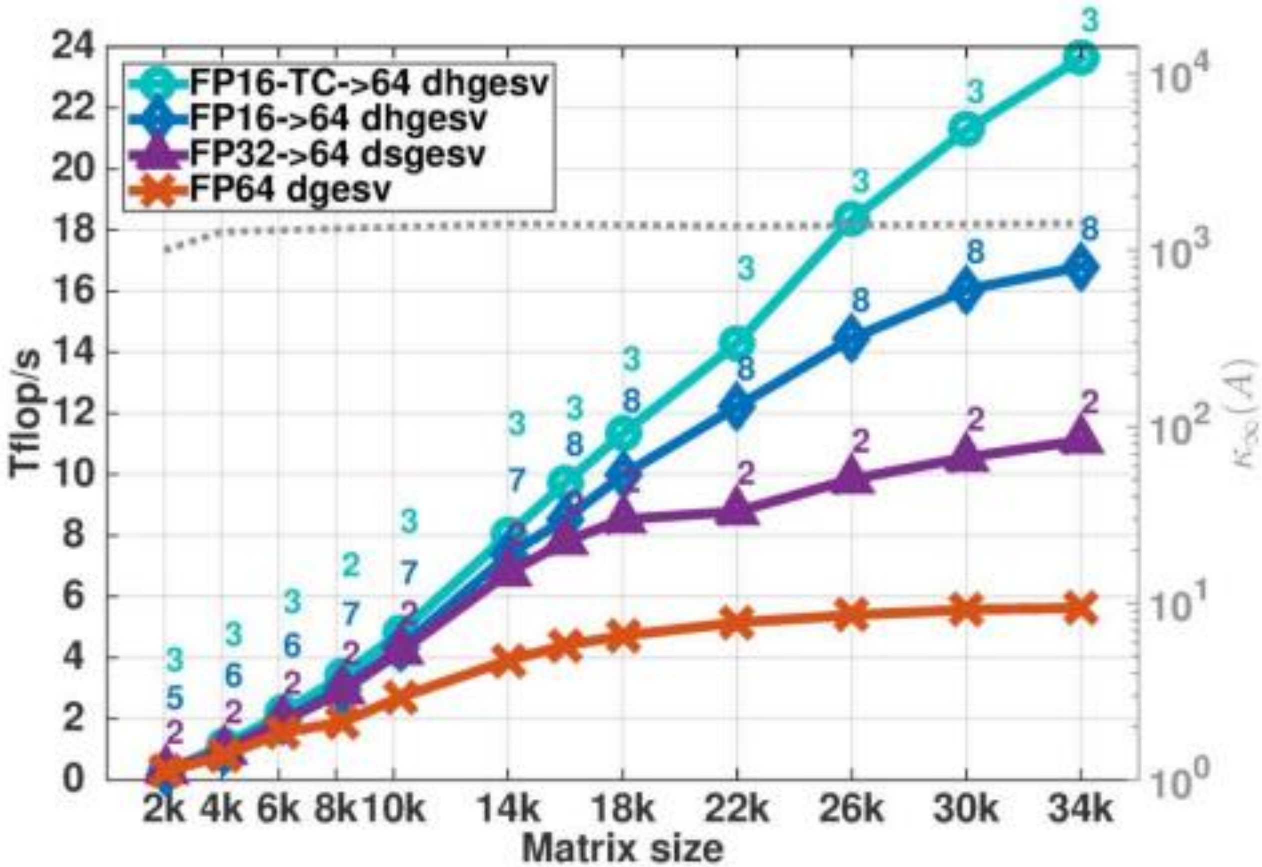
- [Haidar, Tomov, Dongarra, Higham, 2018]
- 2-precision GMRES-IR approach $(u = u_r)$ on NVIDIA V100
- IR run to FP64 accuracy, max 400 iterations in GMRES
- Tflops/s measured as $(2n^3/3)$/time



(a) Matrix of type 1: diagonally dominant.

Performance Results (MAGMA)

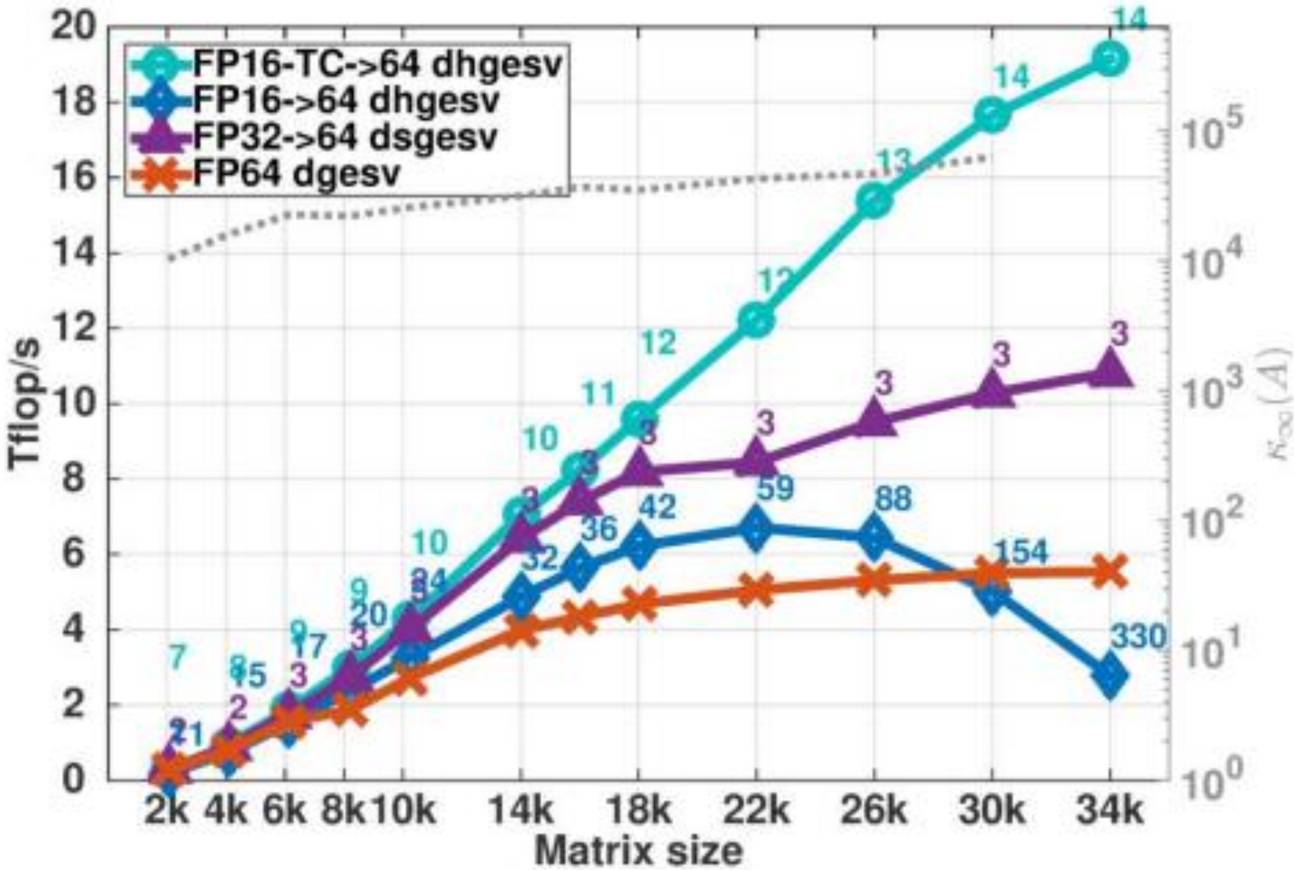
- [Haidar, Tomov, Dongarra, Higham, 2018]



(a) Matrix of type 3: positive λ with clustered singular values, σ_i=(1, $\cdots$, 1, $\frac{1}{cond}$).

Performance Results (MAGMA)

- [Haidar, Tomov, Dongarra, Higham, 2018]



(b) Matrix of type 4: clustered singular values, $\sigma_i = (1, \cdots, 1, \frac{1}{cond})$.

Performance Results

[Haidar, Tomov, Dongarra, Higham, 2018]

Performance for Matrices from SuiteSparse

name	Description	size	$\kappa_\infty(A)$	dgesv	dsgesv		dhgesv		dhgesv-TC		
				time(s)	# iter	time (s)	# iter	time (s)	# iter	time (s)	
em192	radar design	26896	10^6	5.70	3	3.11	40	5.21	10	2.05	2.8×
appu	NASA app benchmark	14000	10^4	0.43	2	0.27	7	0.24	4	0.19	2.3×
ns3Da	3D Navier Stokes	20414	$7.6\ 10^3$	1.12	2	0.69	6	0.54	4	0.43	2.6×
nd6k	ND problem set	18000	$3.5\ 10^2$	0.81	2	0.45	4	0.36	3	0.30	2.7×
nd12k	ND problem set	36000	$4.3\ 10^2$	5.36	2	2.75	3	1.76	3	1.31	4.1×

HPL-AI Benchmark

- HPL/LINPACK benchmark has been used in TOP500 since the 90s
  - Double precision, dense Ax=b using GEPP
  - Not necessarily indicative of application performance, especially for ML/AI applications
  - Doesn't take advantage of low-precision hardware!

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- HPL-AI benchmark (2019)
  - Highlights confluence of HPC+AI workloads
  - Like HPL, solves dense Ax=b, results still to double precision accuracy
  - Achieves this via mixed-precision GMRES-IR
    - may be implemented in a way that takes advantage of the current and upcoming devices for accelerating AI workloads

HPL-AI Benchmark Performance

HPL-AI Results (June 2021):

1. Fugaku: 2 EXAFLOP/s (vs. 442 PETAFLOP/s on HPL; 4.5×)
2. Summit: 1.15 EXAFLOP/s (vs. 149 PETAFLOP/s on HPL; 7.7×)

HPL-AI Benchmark

- In the future, HPL-AI will gain same status as benchmarks that complement HPL, like HPCG, Graph500, Green500
- Usage is growing:
  - 1 machine (2019), 5 machines (2020), 11 machines (2021)
- More information: https://icl.bitbucket.io/hpl-ai/
- Reference implementation: https://bitbucket.org/icl/hpl-ai/src/

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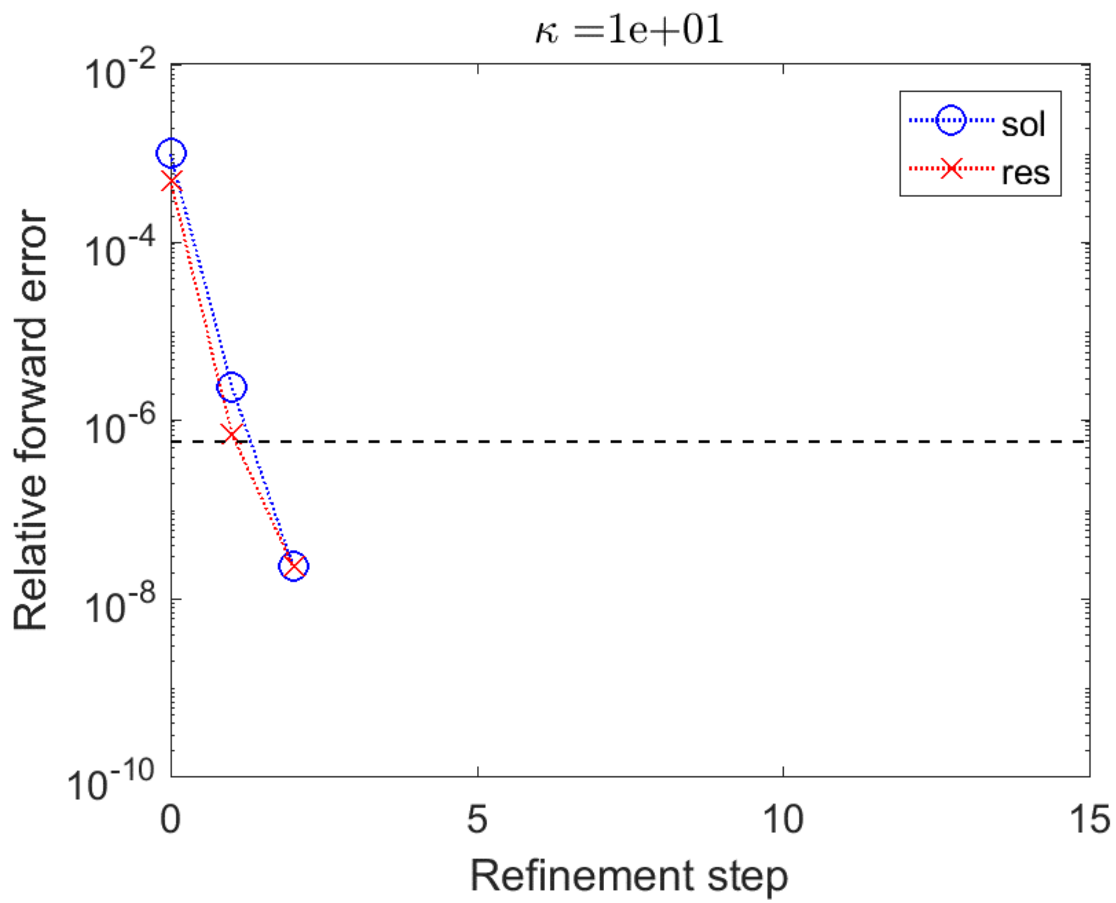
Results for 3-precision IR for linear systems **also applies to least squares problems**

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

(m = 100, n = 10)

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



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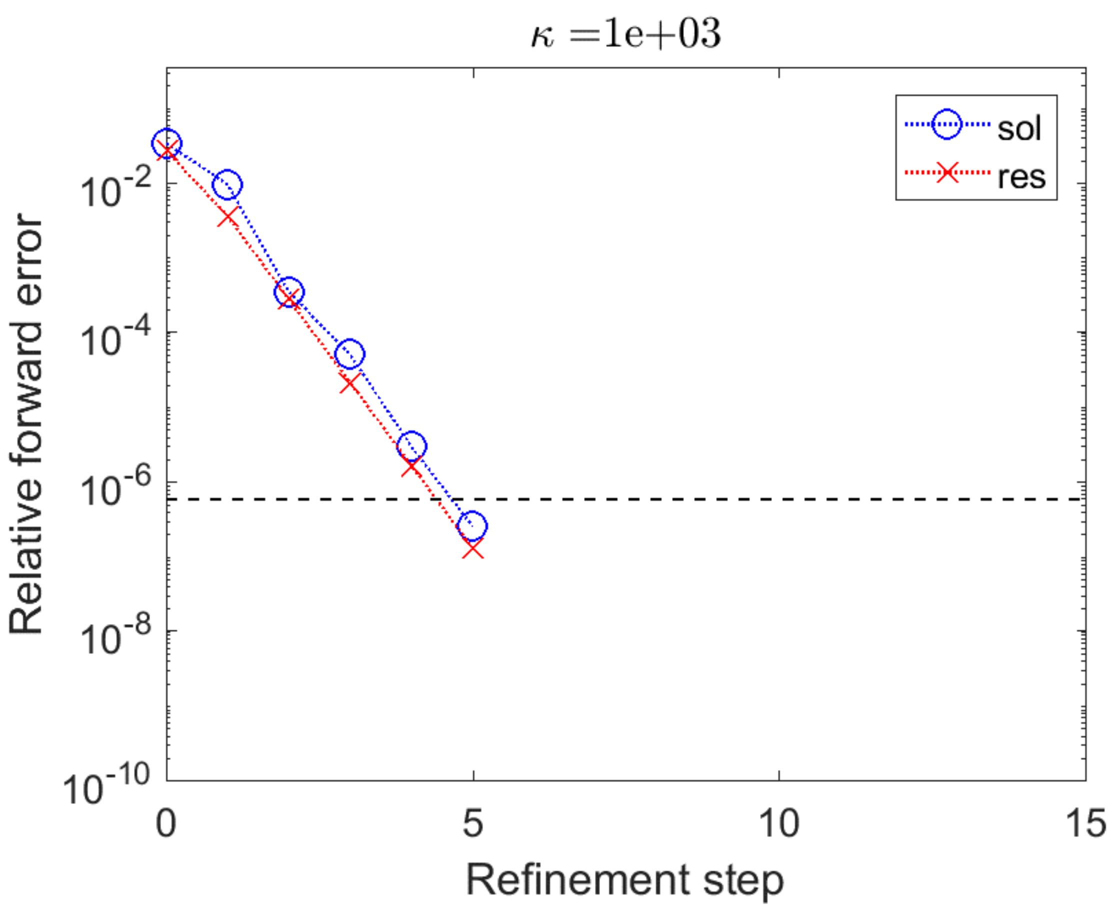

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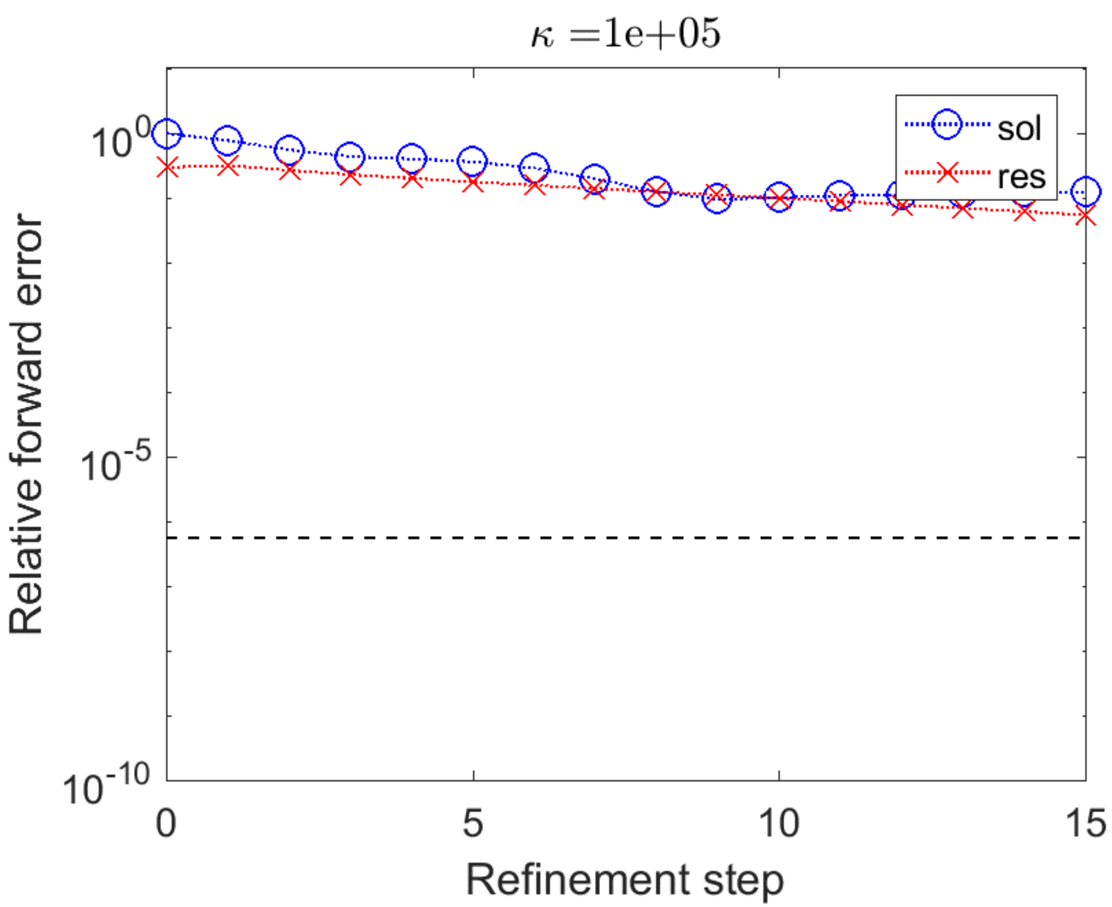

GMRES-IR for Least Squares

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

[C., Higham, Pranesh, SISC 2020]

Further Extensions

- Multistage mixed precision iterative refinement [Oktay, C., 2021]
- Other variants of least squares: underdetermined LS, total LS, data LS
- Use of inexact preconditioners: ILU, SPAI, etc.

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

Mixed precision in NLA

- Iterative refinement:
  - Long history: [Wilkinson, 1963], [Moler, 1967], [Stewart, 1973], ...
  - More recently: [Langou et al., 2006], [C., Higham, 2017], [C., Higham, 2018], [C., Higham, Pranesh, 2020], [Amestoy et al., 2021]
- BLAS: cuBLAS, MAGMA, [Agullo et al. 2009], [Abdelfattah et al., 2019], [Haidar et al., 2018]
- Matrix factorizations: [Haidar et al., 2017], [Haidar et al., 2018], [Haidar et al., 2020], [Abdelfattah et al., 2020]
- Eigenvalue problems: [Dongarra, 1982], [Dongarra, 1983], [Tisseur, 2001], [Davies et al., 2001], [Petschow et al., 2014], [Alvermann et al., 2019]
- Sparse direct solvers: [Buttari et al., 2008]
- Orthogonalization: [Yamazaki et al., 2015]
- Multigrid: [Tamstorf et al., 2020], [Richter et al., 2014], [Sumiyoshi et al., 2014], [Ljungkvist, Kronbichler, 2017, 2019]
- (Preconditioned) Krylov subspace methods: [Emans, van der Meer, 2012], [Yamagishi, Matsumura, 2016], [C., Gergelits, Yamazaki, 2021], [Clark, 2019], [Anzt et al., 2019], [Clark et al., 2010], [Gratton et al., 2020], [Arioli, Duff, 2009], [Hogg, Scott, 2010]

For survey and references, see [Abdelfattah et al., IJHPC, 2021]

Thank You!

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