Mixed Precision Randomized Preconditioners

Erin C. Carson

Charles University

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FACULTY
OF MATHEMATICS
AND PHYSICS
Charles University

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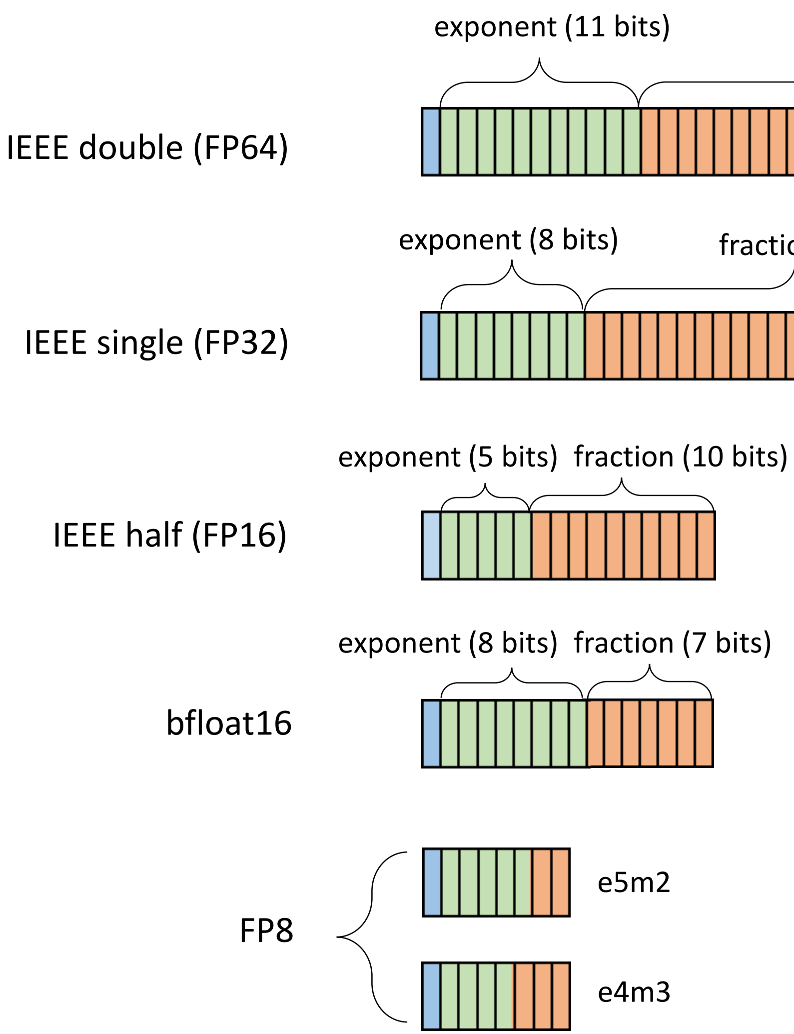
Floating Point Formats

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



	size (bits)	range	u	perf. (NVIDIA H100)
FP64	64	$10^{\pm 308}$	1×10^{-16}	60 Tflops/s
FP32	32	$10^{\pm 38}$	6×10^{-8}	1 Pflop/s
FP16	16	$10^{\pm 5}$	5×10^{-4}	2 Pflops/s
bfloat16	16	$10^{\pm 38}$	4×10^{-3}	
FP8-e5m2	8	$10^{\pm 5}$	1×10^{-1}	4 Pflops/s
FP8-e4m3	8	$10^{\pm 2}$	6×10^{-2}	

Mixed precision in NLA

- BLAS: cuBLAS, MAGMA, [Agullo et al. 2009], [Abdelfattah et al., 2019], [Haidar et al., 2018]
- 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]
- 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], [Higham and Mary, 2022]

HPL-MxP Benchmark

- Supercomputers traditionally ranked by performance on high-performance LINPACK (HPL) benchmark
  - Solves dense $Ax = b$ via Gaussian elimination with partial pivoting

- HPL-MxP: Like HPL, solves dense $Ax = b$, results still to double precision accuracy
  - But achieves this via mixed-precision iterative refinement

HPL-MxP Benchmark

November 2022

Rank	Site	Computer	Cores	HPL-AI (Eflop/s)	TOP500 Rank	HPL Rmax (Eflop/s)	Speedup
1	DOE/SC/ORNL	Frontier	8,730,112	7.942	1	1.1020	7.2
2	EuroHPC/CSC	LUMI	2,174,976	2.168	3	0.3091	7.0
3	RIKEN	Fugaku	7,630,848	2.000	1	0.4420	4.5
4	EuroHPC/CINECA	Leonardo	1,463,616	1.842	4	0.1682	11.0
5	DOE/SC/ORNL	Summit	2,414,592	1.411	2	0.1486	9.5
6	NVIDIA	Selene	555,520	0.630	6	0.0630	9.9
7	DOE/SC/LBNL	Perlmutter	761,856	0.590	5	0.0709	8.3
8	FZJ	JUWELS BM	449,280	0.470	8	0.0440	10.0
9	GENCI-CINES	Adastra	319,072	0.303	11	0.0461	6.6
10	Pawsey Supercomputing Centre	Setonix - GPU	181,248	0.175	15	0.0272	6.4

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When Can I Use Low Precision?

1. When low accuracy is needed

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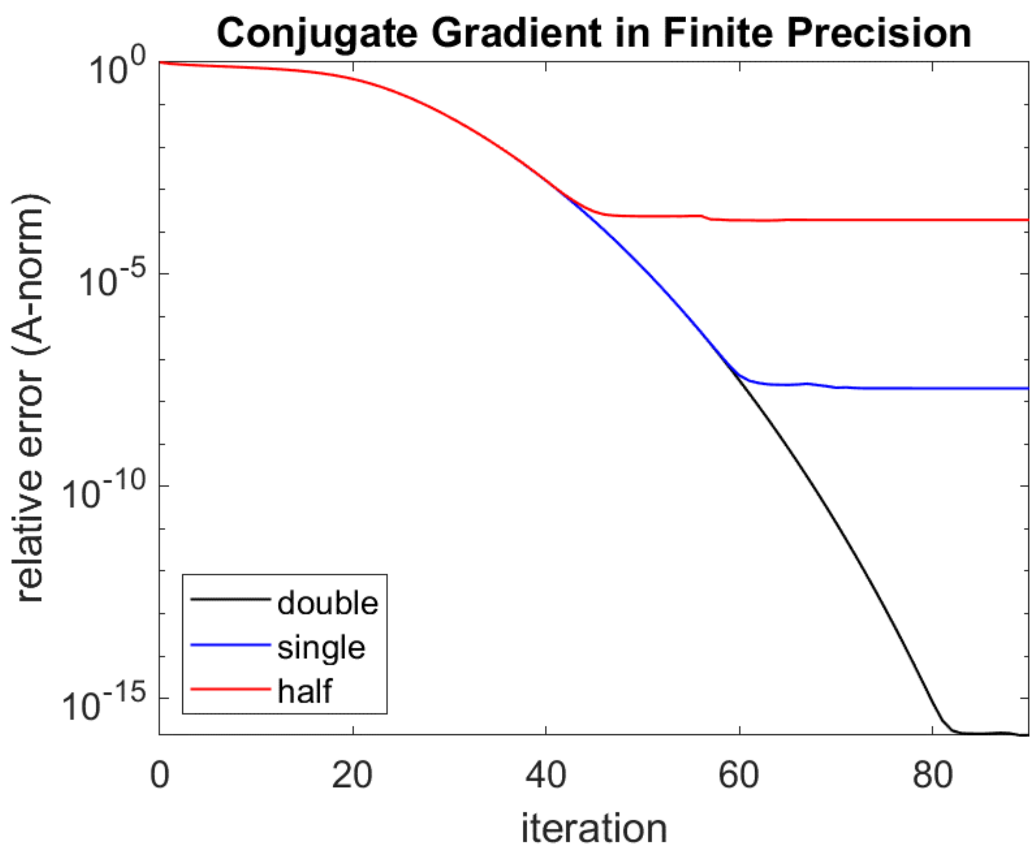
```
A = diag(linspace(.001,1,100));
b = ones(n,1);
```



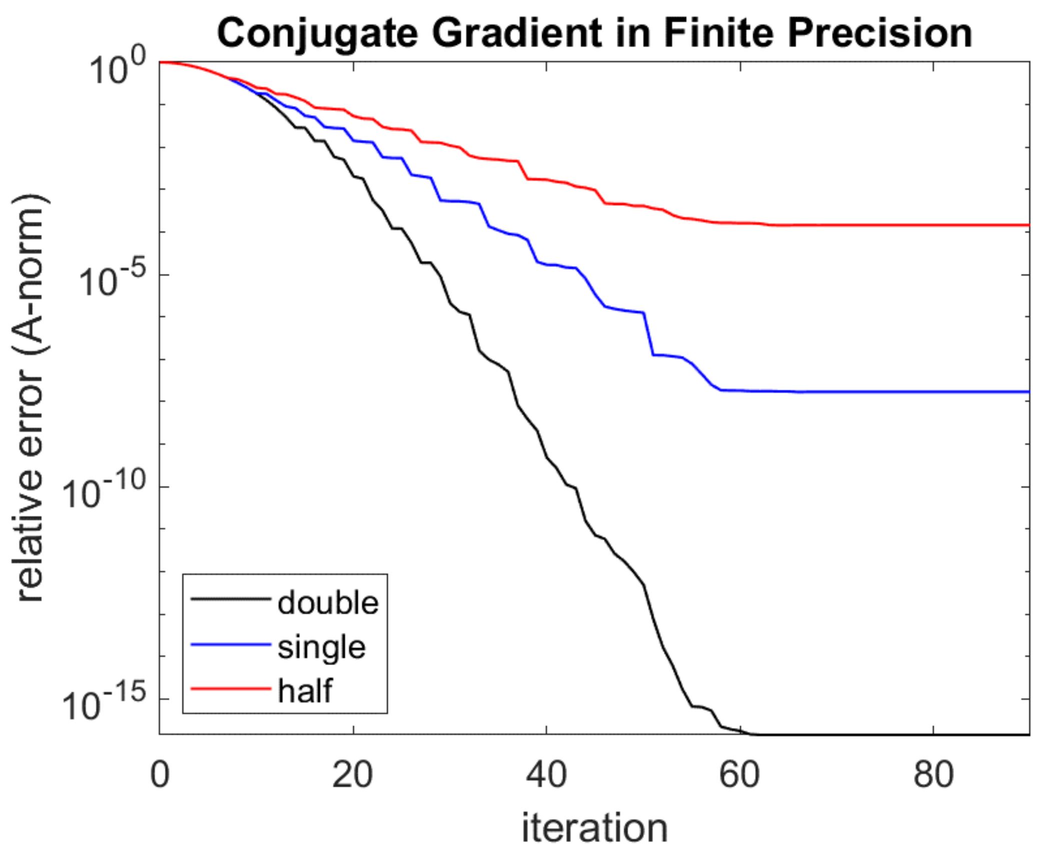
When Can I Use Low Precision?

1. When low accuracy is needed

$n = 100, \lambda_1 = 10^{-3}, \lambda_n = 1$

$\lambda_i = \lambda_1 + \left(\frac{i-1}{n-1}\right)(\lambda_n - \lambda_1)(0.65)^{n-i}, \quad i = 2, \dots, n-1$

```
b = ones(n,1);
```



When Can I Use Low Precision?

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2. When a self-correction mechanism is available

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Example: Iterative refinement

Solve $Ax_0 = b$ by LU factorization (in precision $\boldsymbol{u_f}$)

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

$r_i = b - Ax_i$ (in precision $\boldsymbol{u_r}$)

Solve $Ad_i = r_i$ (in precision $\boldsymbol{u_s}$)

$x_{i+1} = x_i + d_i$ (in precision $\boldsymbol{u}$)

e.g., [Langou et al., 2006], [Arioli and Duff, 2009], [Hogg and Scott, 2010], [Abdelfattah et al., 2016], [C. and Higham, 2018], [Amestoy et al., 2021]

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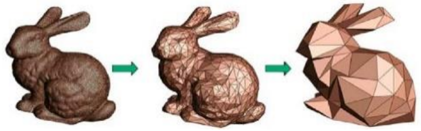
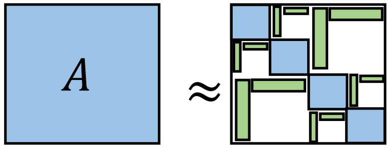
- E.g., reduced models, sparsification, low-rank approximations, randomization

Model Reduction

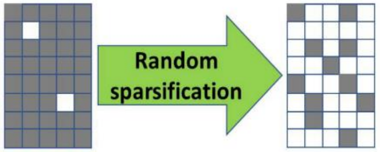


[Schilders, van der Vorst, Rommes, 2008]

Low-rank approximation



Sparsification, randomization



[Sinha, 2018]

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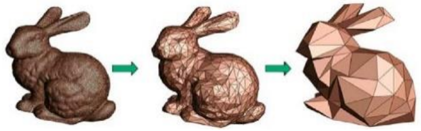

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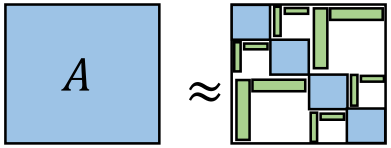
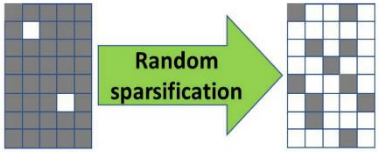


Sparsification, randomization



[Sinha, 2018]

Our setting

Let $A \in \mathbb{R}^{n \times n}$ be a symmetric positive semidefinite matrix. Want to solve

$$(A + \mu I)x = b$$

where $\mu \geq 0$ is set so that $A + \mu I$ is positive definite.

Assume A has rapidly decreasing eigenvalues or cluster of large eigenvalues.

Many applications, e.g., ridge regression.

Limited Memory Preconditioners

Want to solve using PCG using **spectral limited memory preconditioner** [Gratton, Sartenaer, Tshimanga, 2011], [Tshimanga et al., 2008]:

$$P = I - UU^T + \frac{1}{\alpha+\mu} U(\Theta + \mu I)U^T$$

$$P^{-1} = I - UU^T + (\alpha + \mu)U(\Theta + \mu I)^{-1}U^T$$

where columns of $\boldsymbol{U} \in \mathbb{R}^{n\times k}$ **are $\boldsymbol{k}$ approximate eigenvectors of $\boldsymbol{A}$** and $U^T U = I$, **$\boldsymbol{\Theta}$ is diagonal with approximations to eigenvalues of $\boldsymbol{A}$**, and $\alpha \geq 0$.

Used in data assimilation [Laloyaux et al., 2018], [Mogensen, Alonso Balmaseda, Weaver, 2012], [Moore et al., 2011], [Daužickaitė, Lawless, Scott, van Leeuwen, 2021]

Randomized Nyström Approximation

Want to compute a rank-k approximation $A \approx U\Theta U^T$ via the randomized Nyström method.

Nyström approximation:

$$A_N = (AQ)(Q^T AQ)^{+}(AQ)^T$$

where Q is an $n \times k$ test matrix (random projection).

In the case that A is very large, matrix-matrix products with A are the bottleneck.

This motivates the single-pass version of the Nyström method.

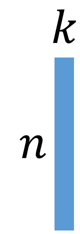
Randomized Nyström Approximation

[Tropp et al., 2017]

Given sym. PSD matrix A, target rank k

$G = \text{randn}(n, k)$

$[Q, \sim] = \text{qr}(G, 0)$



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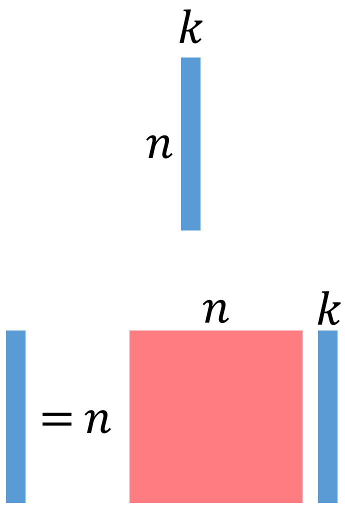

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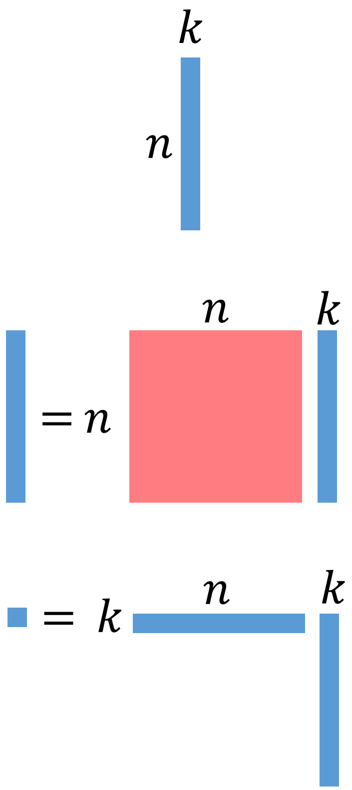
$\boldsymbol{Y} = \boldsymbol{AQ}$

Compute shift ν; $Y_\nu = Y + \nu Q$

$B = Q^T Y_\nu$



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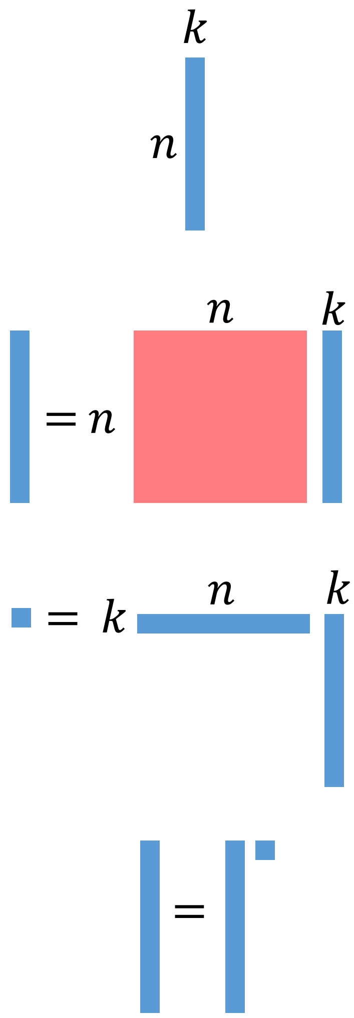
$B = Q^T Y_\nu$

$C = \text{chol}((B + B^T)/2)$

Solve $F = Y_\nu / C$



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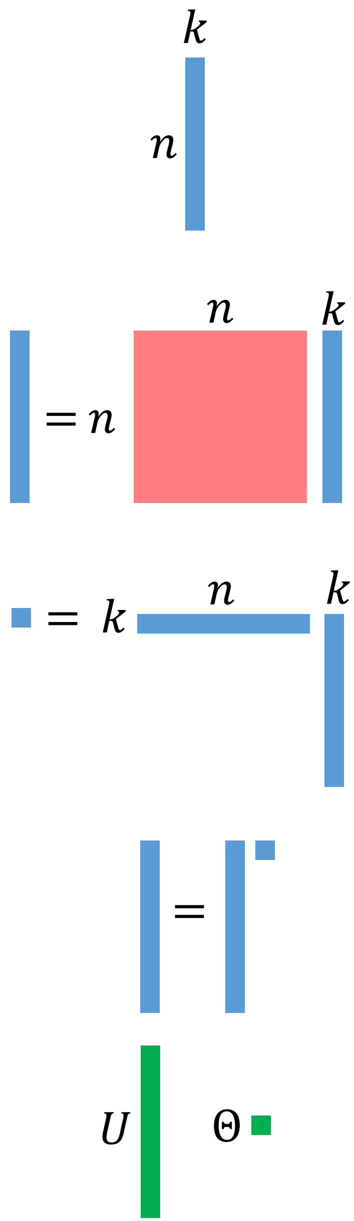
$[U, \Sigma, \sim] = \text{svd}(F, 0)$

$\Theta = \max(0, \Sigma^2 - \nu I)$



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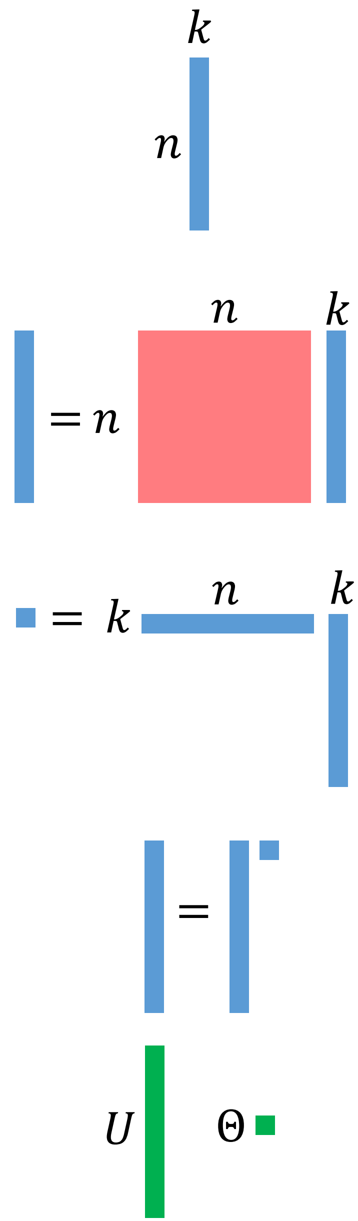
Can we further reduce the cost of the matrix-matrix product with A by using low precision?



Error Bounds

$$\left\|A - \hat{A}_N\right\|_2 = \left\|A - A_N + A_N - \hat{A}_N\right\|_2 \leq \|A - A_N\|_2 + \left\|A_N - \hat{A}_N\right\|_2$$

exact Nyström approximation

Nyström approximation computed in finite precision

Error Bounds

$$\left\|A - \hat{A}_N\right\|_2 = \left\|A - A_N + A_N - \hat{A}_N\right\|_2 \leq \underbrace{\|A - A_N\|_2}_{\text{exact approximation error}} + \underbrace{\left\|A_N - \hat{A}_N\right\|_2}_{\text{finite precision error}}$$

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Deterministic bound [Gittens, Mahoney, 2016]:

$$\|A - A_N\|_2 \leq \lambda_{k+1} + \left\|\Sigma_2^{1/2} U_2^T Q (U_1 Q)^+\right\|_2^2$$

with $A = [U_1 \;\; U_2] \begin{bmatrix} \Sigma_1 & \\ & \Sigma_2 \end{bmatrix} [U_1 \; U_2]^T$.

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Expected value bound [Frangella, Tropp, Udell, 2021]:

$$\mathbb{E}\|A - A_N\|_2 \leq \min_{2 \leq p \leq k-2} \left(\left(1 + \frac{2(k-p)}{p-1}\right) \lambda_{k-p+1} + \frac{2e^2 k}{p^2 - 1} \sum_{j=k-p+1}^{n} \lambda_j \right)$$

where $\lambda_i \geq \lambda_{i+1}$ are the eigenvalues of A.

Finite Precision Error Bound

Finite precision error: $A_N - \hat{A}_N$

Assumptions:

- A is stored in precision u_p and matrix-matrix product AQ is computed in precision u_p
- All other quantities stored and computed in precision $u \ll u_p$

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[C., Daužickaitė, 2022]: With failure probability at most $e^{-t^2/2} + c_1\alpha$,

$$\left\|A_N - \hat{A}_N\right\|_2 \lesssim \alpha^{-1} n^{1/2} k \left(n^{1/2} + k^{1/2} + t\right)^2 u_p \|A\|_2 \kappa(A_k)$$

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Interpretation: Likely that $\left\|A_N - \hat{A}_N\right\|_2 \gtrsim \|A - A_N\|_2$ when

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The more approximate the low-rank representation, the lower the precision we can use!

Condition Number Bounds

Let $E = A - A_N$, $\mathcal{E} = A_N - \hat{A}_N$, and assume $(A + \mu I)$ is SPD.

Let

$$\hat{P}^{-1} = I - \widehat{U}\widehat{U}^T + \left(\hat{\lambda}_k + \mu\right)\widehat{U}\left(\widehat{\Theta} + \mu I\right)^{-1}\widehat{U}^T$$

be the LMP preconditioner constructed using the mixed precision Nyström approximation $\hat{A}_N = \widehat{U}\widehat{\Theta}\widehat{U}^T$.

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Then

$$\max\left\{1, \frac{\hat{\lambda}_k + \mu - \|\mathcal{E}\|_2}{\mu + \lambda_{min}(A)}\right\} \leq \kappa\left(\hat{P}^{-1/2}(A + \mu I)\hat{P}^{-1/2}\right) \leq 1 + \frac{\hat{\lambda}_k + \|E\|_2 + 2\|\mathcal{E}\|_2}{\mu - \|\mathcal{E}\|_2}$$

where the upper bound holds if $\mu > \|\mathcal{E}\|_2$.

Regardless of this constraint, if A is positive definite, then

$$\kappa\left(\hat{P}^{-1/2}(A + \mu I)\hat{P}^{-1/2}\right) \leq \left(\hat{\lambda}_k + \mu + \|E\|_2 + \|\mathcal{E}\|_2\right)\left(\frac{1}{\hat{\lambda}_k + \mu} + \frac{\|\mathcal{E}\|_2 + 1}{\lambda_{min}(A) + \mu}\right).$$

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be the LMP preconditioner constructed using the mixed precision Nyström approximation $\hat{A}_N = \widehat{U}\widehat{\Theta}\widehat{U}^T$.

If $\mathcal{E} = 0$, reduces to bounds of [Frangella, Tropp, Udell, 2021] for exact case.

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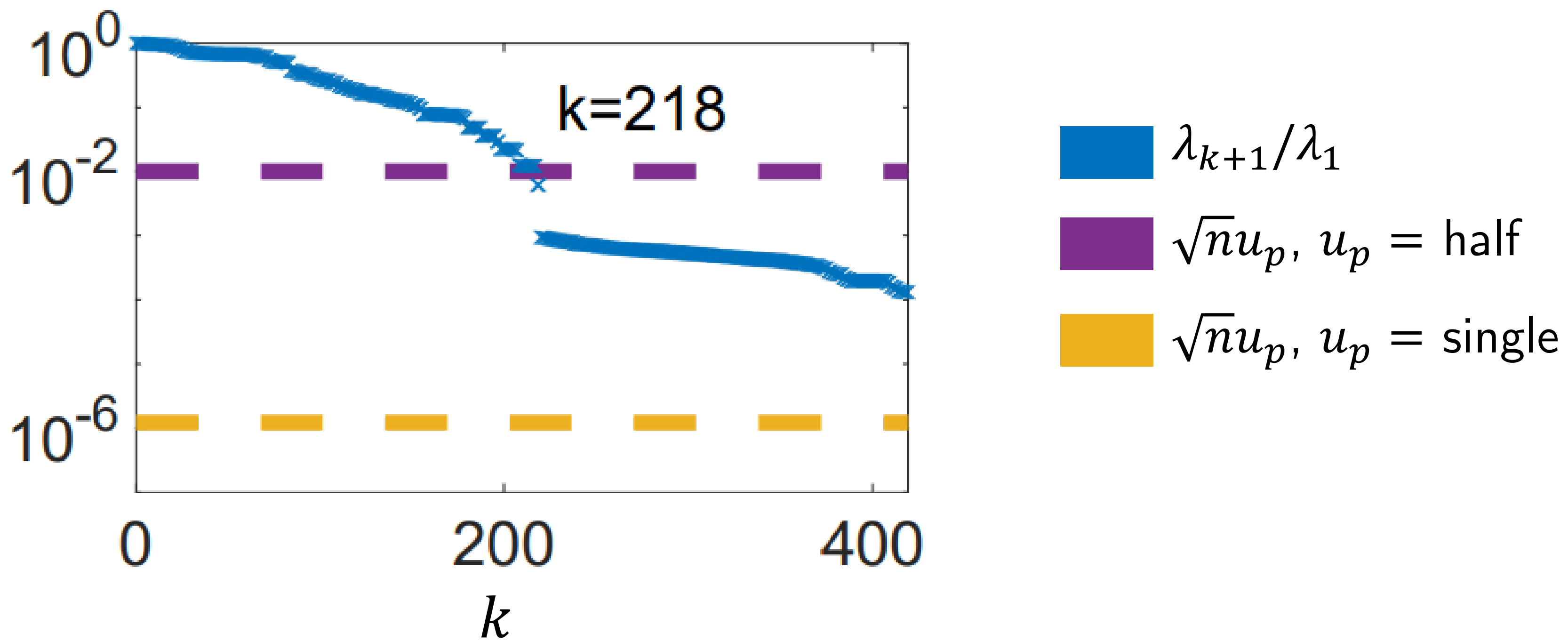
Numerical Experiment

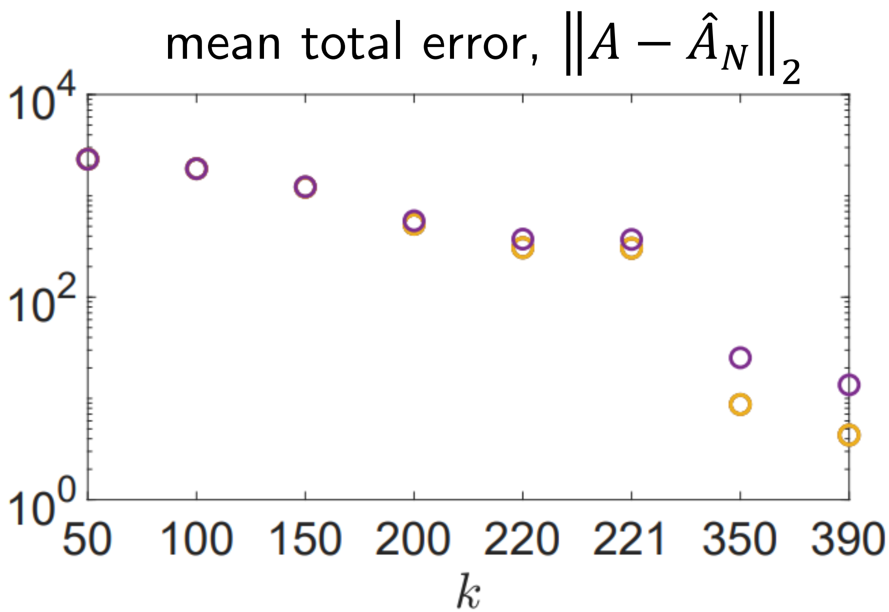
Matrix: bcsstm07, $n = 420$

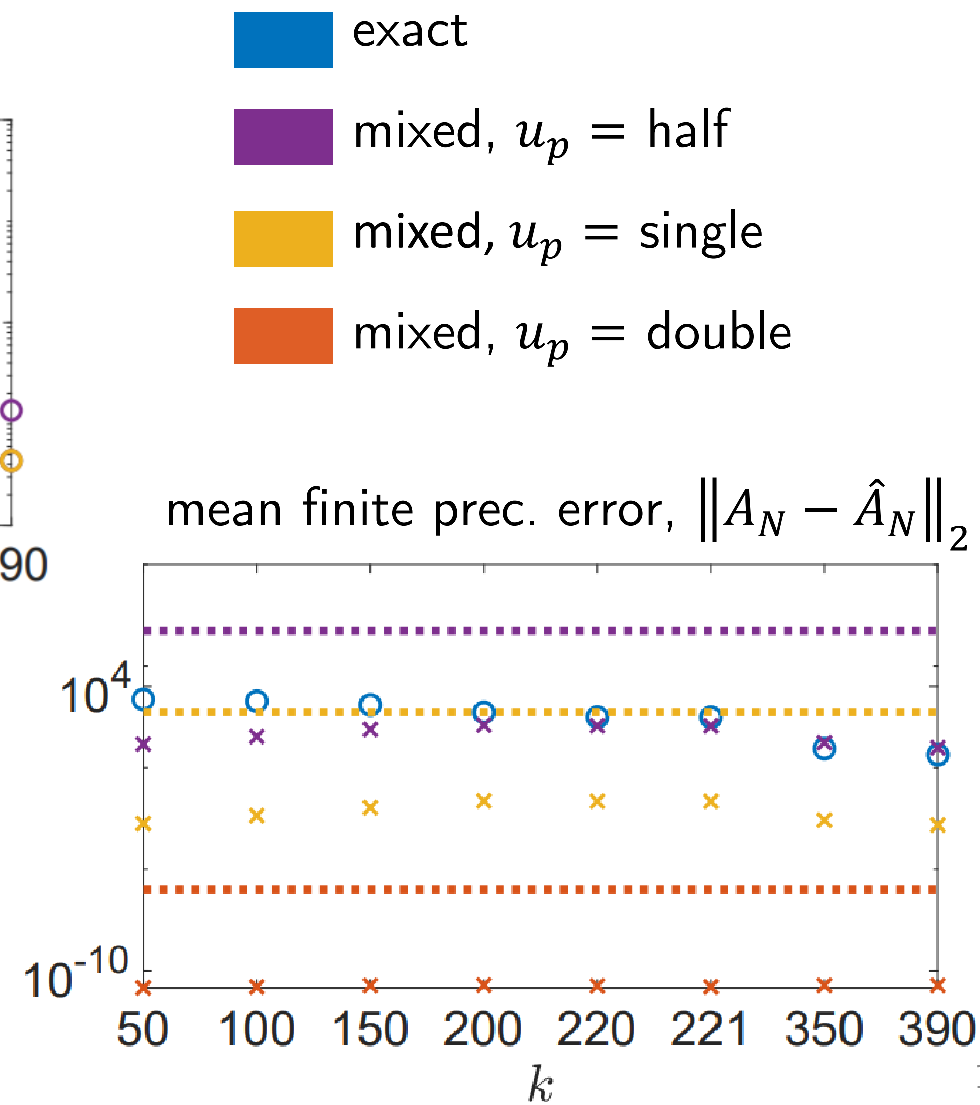


https://github.com/dauzickaite/mpNystrom

Numerical Experiment

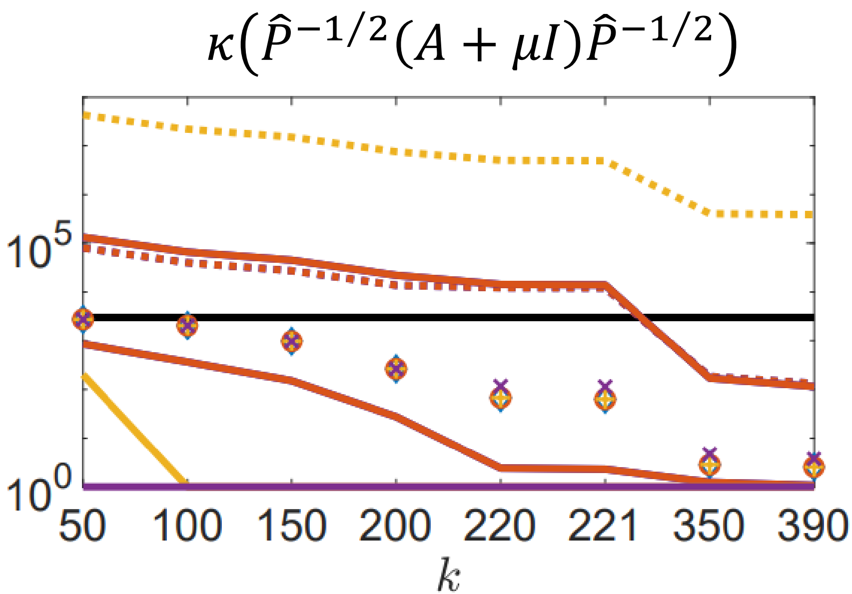
Matrix: bcsstm07, $n = 420$

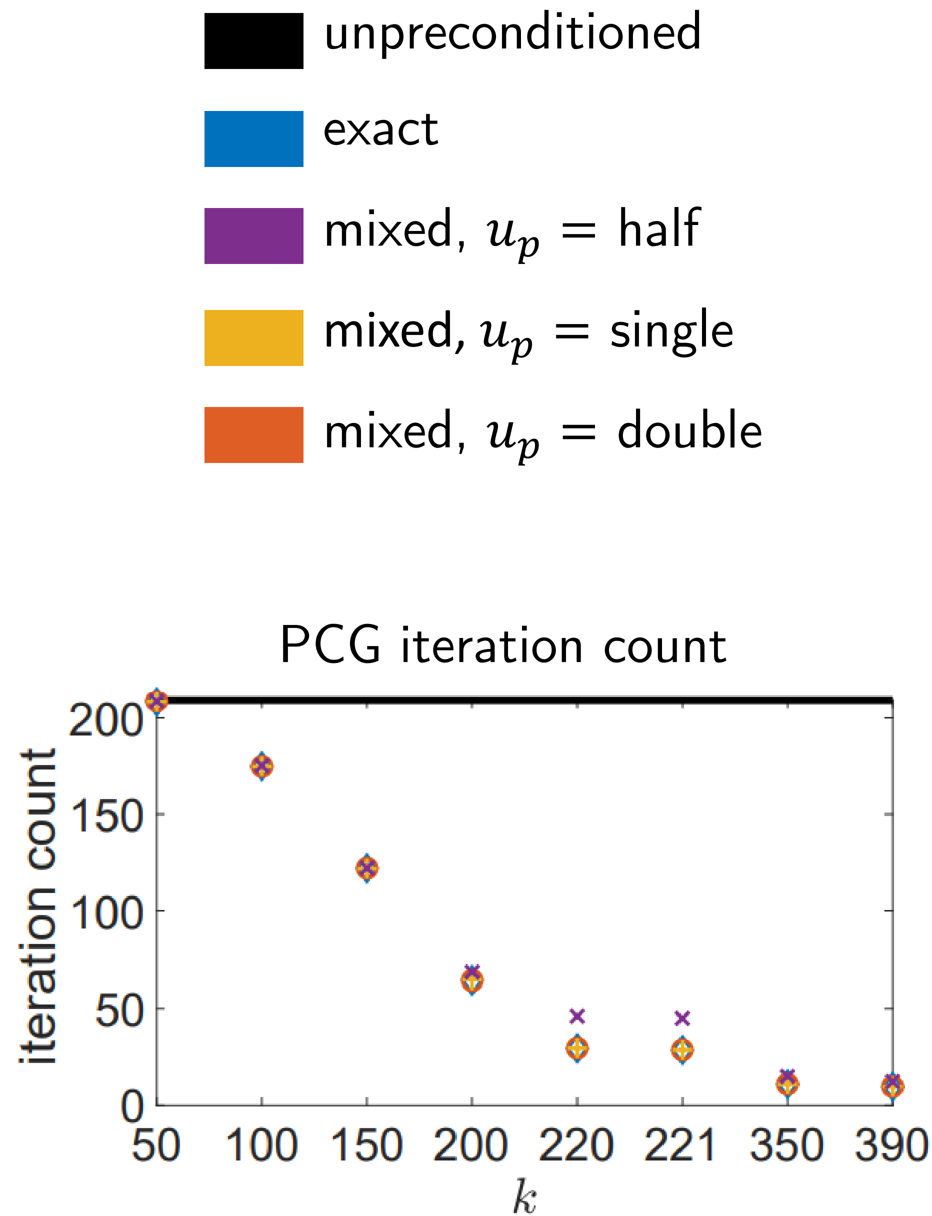




https://github.com/dauzickaite/mpNystrom

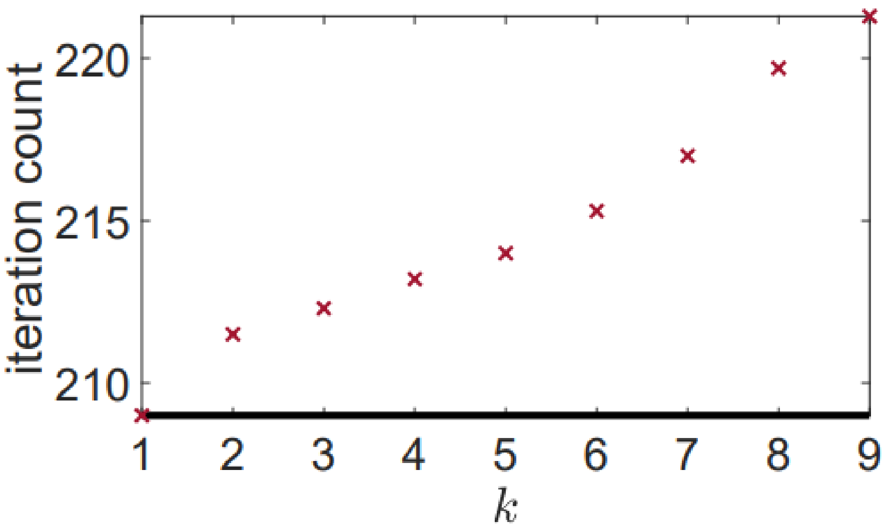
Numerical Experiment



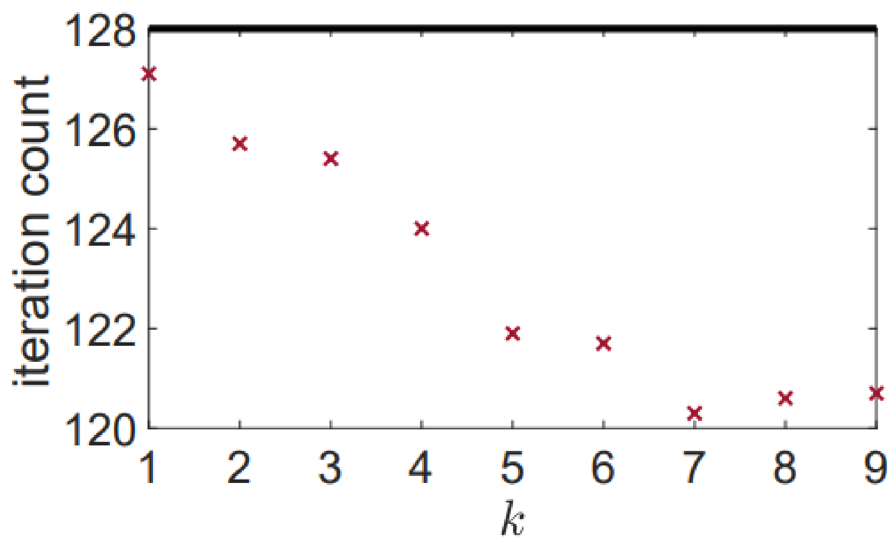


https://github.com/dauzickaite/mpNystrom

Quarter precision?



bcsstm07, iteration count



Journals, iteration count

https://github.com/dauzickaite/mpNystrom

Summary and Takeaway

- We now have a multi-precision ecosystem
- Huge opportunities for using mixed precision in matrix computations
- But also big challenges!

Thank You!

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