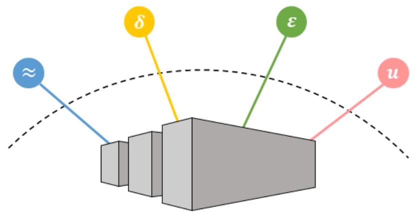

Forward and backward error bounds for a mixed precision preconditioned conjugate gradient algorithm

Thomas Bake[1], Erin Carson[1], Yuxin Ma[1].

HPCSE 2026 - Hotel Solaň

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[1]Charles University

Contributions

1. General framework for preconditioned conjugate gradient (PCG).

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2. Forward and backward error bounds for PCG.

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2. Forward and backward error bounds for PCG.
3. Extension of bounds to incorporate mixed precision.

The conjugate gradient method

CG method

- $Ax = b$, $A \in \mathbb{R}^{n\times n}$ symmetric positive definite (SPD), large and sparse, $b \in \mathbb{R}^n$.

Algorithm 1: The CG algorithm

$r_0 = b - Ax_0, \quad p_0 = r_0$

for $k = 0, 1, \dots, n_{\max}$

  $\alpha_k = \frac{r_k^\top r_k}{p_k^\top A p_k}$

  $x_{k+1} = x_k + \alpha_k p_k$

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  Stop when stopping criterion is satisfied

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CG method

- $Ax = b, \quad A \in \mathbb{R}^{n\times n}$ symmetric positive definite (SPD), large and sparse, $b \in \mathbb{R}^n$.

- Mathematically, the *residual* vectors

$$r_0, r_1, \dots, r_k$$

and the *direction* vectors

$$p_0, p_1, \dots, p_k$$

form orthogonal bases of $\mathcal{K}_k(A, r_0)$ with respect to the Euclidean and A-inner products, respectively.

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$r_0 = b - Ax_0, \quad p_0 = r_0$
for $k = 0, 1, \dots, n_{\max}$
  $\alpha_k = \frac{r_k^T r_k}{p_k^T A p_k}$
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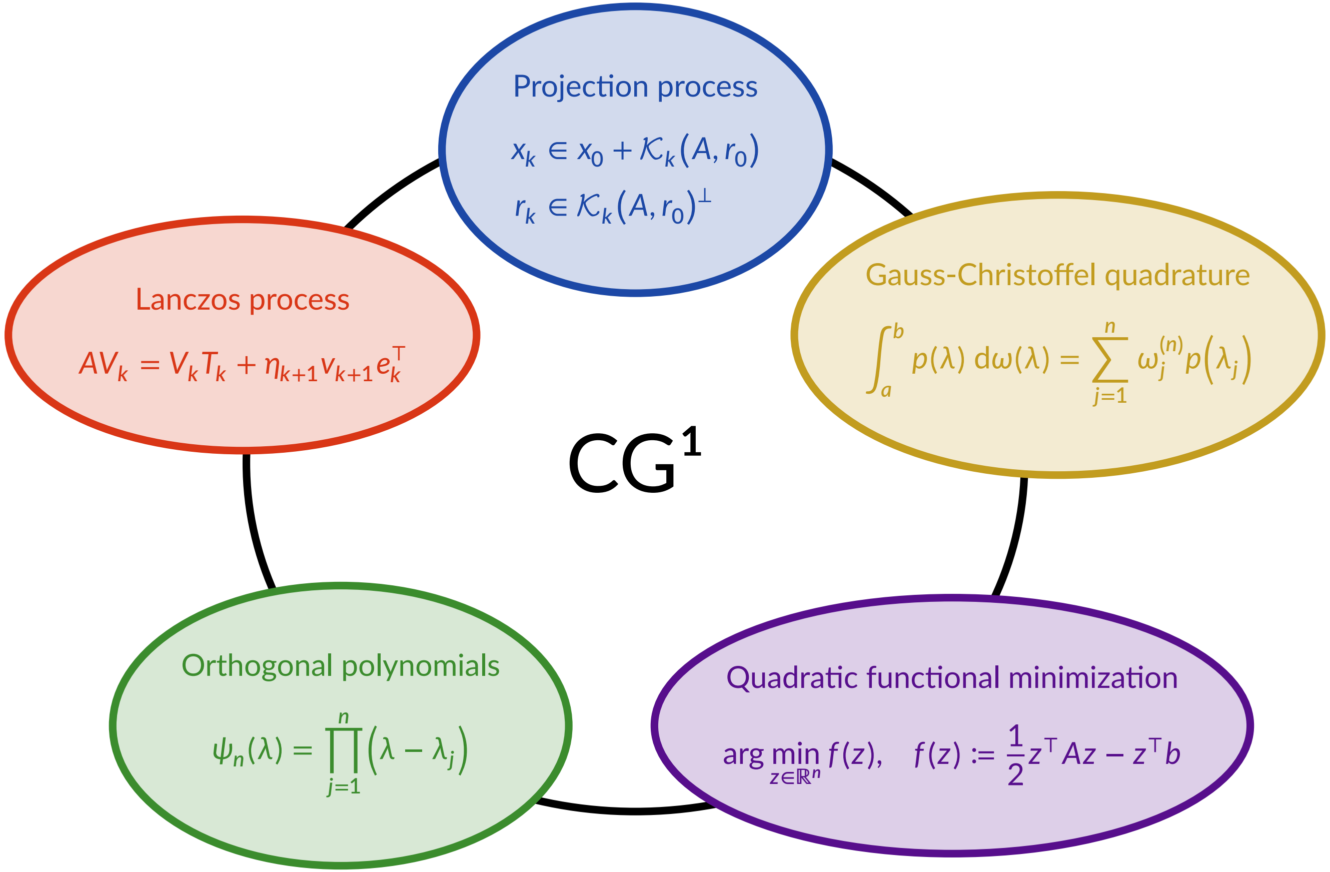
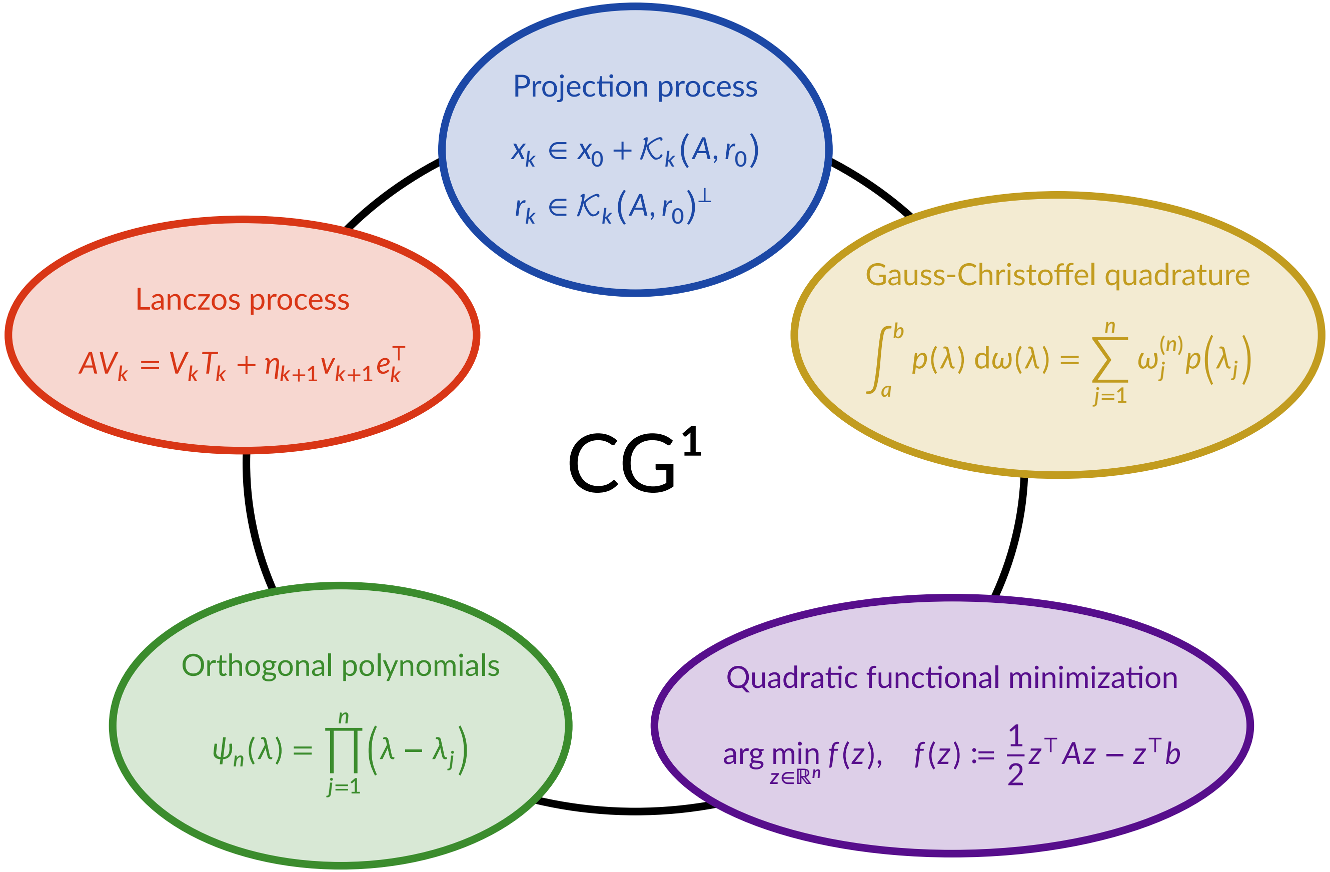


[1]Idea of graphic taken from Petr Tichý.

CG method



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Preconditioned conjugate gradient

Preconditioning and PCG

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$$\xrightarrow[M = M_L \cdot M_R \in \mathbb{R}^{n\times n}]{\text{SPD preconditioner}}$$

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SPD preconditioner

$\longrightarrow$

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$r_0 = b - Ax_0, \quad s_0 = M_L^{-1} r_0, \quad q_0 = M_R^{-1} s_0,$
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- $M_L^{-1} A M_R^{-1}$ must be SPD with respect to an inner product.

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- Example: Let $M = LL^\top$ be the Cholesky factorization of M.

Scheme		
Left	$M_L = LL^\top$	$M_R = I_n$
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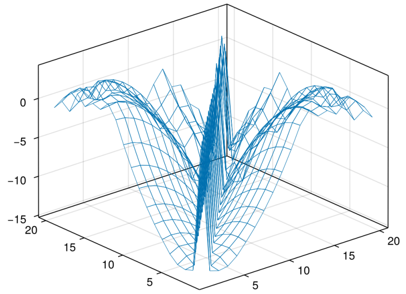
What can we say about this algorithm in *finite precision*?

Forward and backward error bounds

$$
\begin{tikzcd}[column sep=huge, row sep=huge]
x \arrow[r, "f"] \arrow[d, "\|\Delta x\|_{\mathcal{X}}"'] & y = f(x) \arrow[d, "\|y - \hat{y}\|_{\mathcal{Y}}"] \\
x + \Delta x \arrow[r, "f"'] & \hat{y} = f(x + \Delta x)
\end{tikzcd}
$$

Previous work on finite precision Lanczos / CG

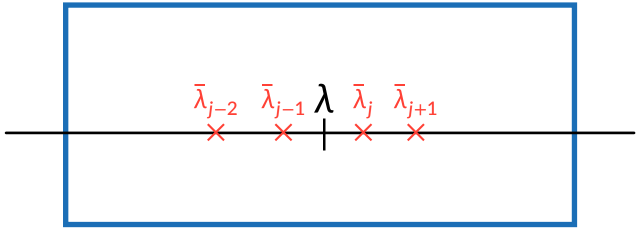
(Paige 1976, 1980)



(Greenbaum 1997)

$$\|b - A\hat{x}_k\| \le \|b - A\hat{x}_k - \hat{r}_k\| + \|\hat{r}_k\| \xrightarrow{\|\hat{r}_k\| \to 0} \|b - A\hat{x}_k - \hat{r}_k\|$$

$$\|b - A\hat{x}_k - \hat{r}_k\| \le O(nk\boldsymbol{u})\,\|A\| \max_{j\le k}\left(\|\hat{x}_j\|, \|x\|\right)$$



(Greenbaum 1989)

$\|\hat{r}_k\| \le ?$

Preliminaries

- Let the symbol $\hat{\cdot}$ denote quantities computed in finite precision. Assume $n\boldsymbol{u} < 1$, where $\boldsymbol{u}$ denotes the unit roundoff.

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$$f(\bar{x}_k) - f(\bar{x}_{k+1}) = -\frac{1}{2}\hat{\alpha}_k(1 + \delta\alpha_k)\|\hat{r}_k\|^2_{M^{-1}} + \delta f_k,$$

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Key result:

$$O(n\boldsymbol{u})\kappa(A) + 2\epsilon_{\text{pre}}^{(s,z)} \le 1/2 \quad \Longrightarrow \quad \exists k^\star \ge 1 : f(\bar{x}_{k^\star}) - f(\bar{x}_{k^\star+1}) \le O\Big[n^2(k^\star)^2\boldsymbol{u}^2\Big]\hat{\alpha}_{k^\star}\|A\|^2\|M^{-1}\|\|x\|^2.$$

Main result[1]

Furthermore, if $k^\star$ satisfies

$$\boxed{\frac{O[n(k^\star+1)\boldsymbol{u}]\kappa(A)}{1-O(n\boldsymbol{u})\kappa(A)} + O(k^\star+1)\left[\epsilon_{\text{pre}}^{(s,q)} + \epsilon_{\text{pre}}^{(s,z)}\right] + O[(k^\star+1)\boldsymbol{u}]\kappa(M)^{\frac{1}{2}}\left[1 + k^\star\kappa\left(M_L^{-1}AM_R^{-1}\right)^{\frac{1}{2}}\right] \le \frac{1}{2},}$$

then there exists an iteration step $i \le k^\star$ such that

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$$\frac{1}{\kappa(A)^{\frac{1}{2}}}\cdot\left[\frac{\|x-\hat{x}_i\|_A}{\|x\|_A}\right] \le \frac{\|x-\hat{x}_i\|_A}{\|A\|^{\frac{1}{2}}\|x\|} \le O\Big[n(k^\star)^2\boldsymbol{u}\Big]\kappa(M)^{\frac{1}{2}}\kappa(A)^{\frac{1}{2}} \max_{j\le k^\star+1}\left(\frac{\|\hat{x}_j\|}{\|x\|}, 1\right).$$

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Remarks:

- Influence of problem size n and iteration steps k are usually *overestimates*.

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Furthermore, if $k^\star$ satisfies

$$\frac{O[n(k^\star+1)\boldsymbol{u}]\kappa(A)}{1-O(n\boldsymbol{u})\kappa(A)} + O(k^\star+1)\left[\epsilon_{\text{pre}}^{(s,q)} + \epsilon_{\text{pre}}^{(s,z)}\right] + O[(k^\star+1)\boldsymbol{u}]\kappa(M)^{\frac{1}{2}}\left[1 + k^\star\kappa\left(M_L^{-1}AM_R^{-1}\right)^{\frac{1}{2}}\right] \le \frac{1}{2},$$

then there exists an iteration step $i \le k^\star$ such that

$$\frac{\|\hat{r}_i\|}{\|A\|\|x\|} \le O\left[n(k^\star)^2\boldsymbol{u}\right]\kappa(M)^{\frac{1}{2}} \max_{j\le k^\star+1}\left(\frac{\|\hat{x}_j\|}{\|x\|}, 1\right),$$

$$\frac{\|\hat{x}_i\|}{\|x\|}\cdot\left[\frac{\|b-A\hat{x}_i\|}{\|A\|\|\hat{x}_i\|+\|b\|}\right] \le \frac{\|b-A\hat{x}_i\|}{\|A\|\|x\|} \le O\left[n(k^\star)^2\boldsymbol{u}\right]\kappa(M)^{\frac{1}{2}} \max_{j\le k^\star+1}\left(\frac{\|\hat{x}_j\|}{\|x\|}, 1\right),$$

$$\frac{1}{\kappa(A)^{\frac{1}{2}}}\cdot\left[\frac{\|x-\hat{x}_i\|_A}{\|x\|_A}\right] \le \frac{\|x-\hat{x}_i\|_A}{\|A\|^{\frac{1}{2}}\|x\|} \le O\left[n(k^\star)^2\boldsymbol{u}\right]\kappa(M)^{\frac{1}{2}}\kappa(A)^{\frac{1}{2}} \max_{j\le k^\star+1}\left(\frac{\|\hat{x}_j\|}{\|x\|}, 1\right).$$

Remarks:

- Influence of problem size n and iteration steps k are usually *overestimates*.
- The iteration step $k^\star$ is *unknown*.

[1](B., Carson, and Ma 2025, Theorem 2)

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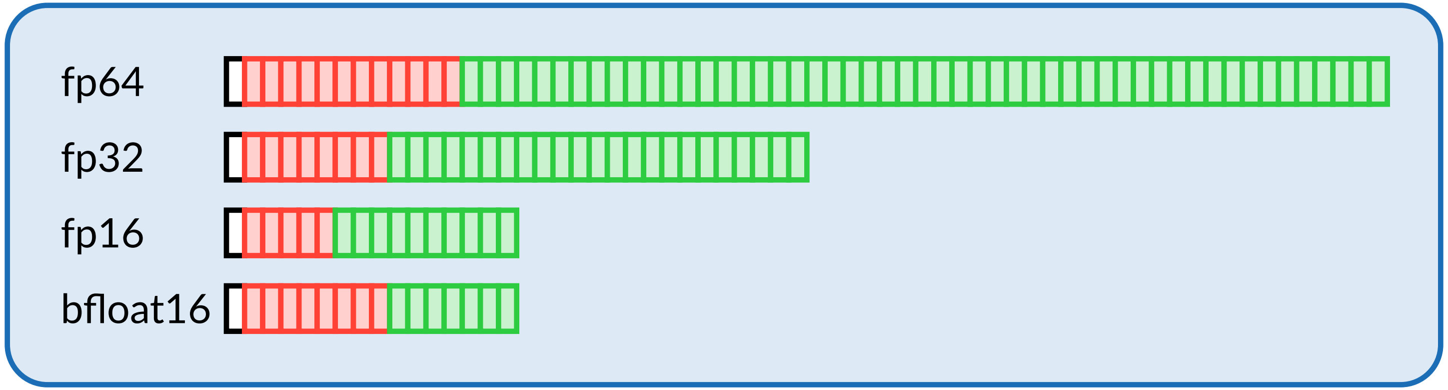
$$\frac{1}{\kappa(A)^{\frac{1}{2}}} \cdot \left[\frac{\|x - \hat{x}_i\|_A}{\|x\|_A}\right] \leq \frac{\|x - \hat{x}_i\|_A}{\|A\|^{\frac{1}{2}}\|x\|} \leq O\left[n(k^\star)^2\boldsymbol{u}\right]\kappa(M)^{\frac{1}{2}}\kappa(A)^{\frac{1}{2}} \max_{j\leq k^\star+1}\left(\frac{\|\hat{x}_j\|}{\|x\|}, 1\right). \tag{3}$$

Remarks:

- Influence of problem size n and iteration steps k are usually *overestimates*.
- The iteration step $k^\star$ is *unknown*.
- Forward and backward errors are small when $f(\bar{x}_k) - f(\bar{x}_{k+1})$ is sufficiently small for some $k \geq 1$.

[1](B., Carson, and Ma 2025, Theorem 2)

Extension to mixed precision



Extension to mixed precision

Main idea: Strategic combination of different computer arithmetics to achieve high accuracy at lower cost.

[1](Carson and Mary 2025)

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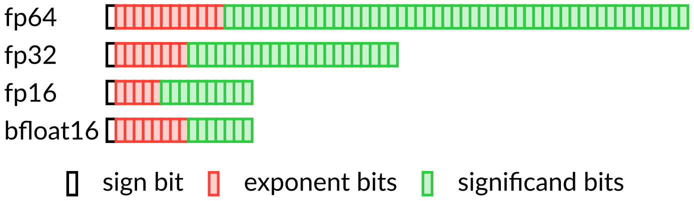

Real world phenomena

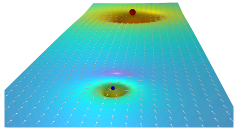

Figure 1: Source: https://www.comsol.com

$\downarrow \varepsilon_m$

Mathematical model — $\nabla^2 \cdot \boldsymbol{g} = -4\pi G\rho$

$\downarrow \varepsilon_d$

Discretization — $\mathcal{V} \to \mathcal{V}_n \subset \mathcal{V}$

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Computation — $Ax = b \to A\hat{x} = b$

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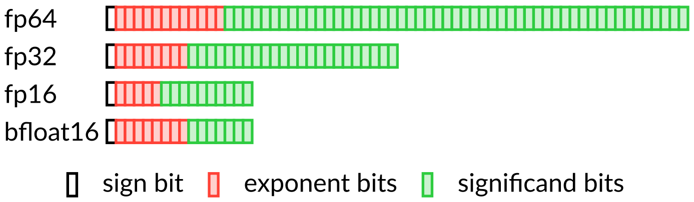

Approach: Perform rounding error analysis and identify precision requirements for different parts of computation.

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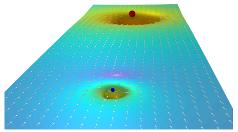

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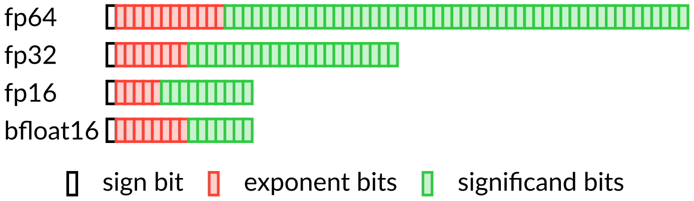

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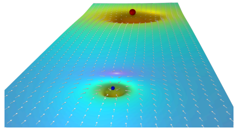

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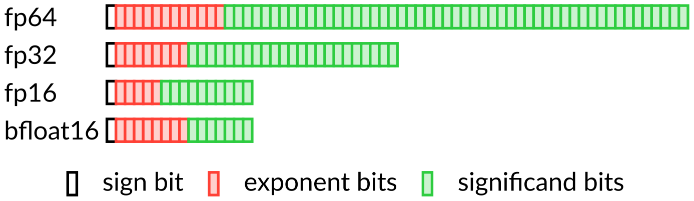

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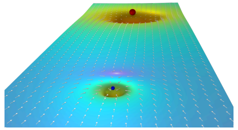

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- **Low precision:** Reduce computation and communication costs.
- **When:**[1] For instance, when the *finite precision error is small* compared to other sources of error.

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Extension to mixed precision

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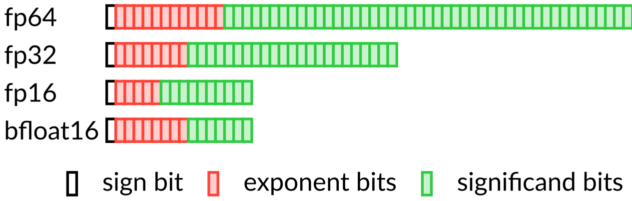

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Our context: Can we apply the preconditioners in *low* precision?

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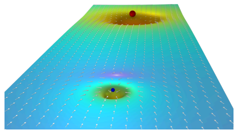

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Mixed precision bounds

Corollary . Let $\boldsymbol{u}_s$, $\boldsymbol{u}_q$, and $\boldsymbol{u}_z$ denote the unit roundoff values associated with the precisions involved in the application of the preconditioners M_L, M_R, and M_R^T, respectively. If $O(n\boldsymbol{u})\kappa(A) + O(n\boldsymbol{u}_1)\kappa(M)^{m_1} \leq \frac{1}{2}$, where

$$\boldsymbol{u}_1 = \begin{cases} \boldsymbol{u}_s & \text{for left PCG,} \\ \boldsymbol{u}_z & \text{for right PCG,} \\ (\boldsymbol{u}_s + \boldsymbol{u}_z) & \text{for split PCG,} \end{cases} \text{ and } \; m_1 = \begin{cases} \frac{3}{2} & \text{for left or right PCG,} \\ \frac{1}{2} & \text{for split PCG,} \end{cases}$$

then there exists an iteration step $k^\star$ such that $f(\bar{x}_{k^\star}) - f(\bar{x}_{k^\star+1}) \leq O\left[n^2(k^\star)^2\boldsymbol{u}^2\right]\hat{\alpha}_{k^\star}\|A\|^2\|M^{-1}\|\|x\|^2$ holds.

Furthermore, if $k^\star$ satisfies

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Main point: If some conditions are met, we can

- potentially apply the preconditioners in *different precisions*, and
- our forward and backward error *bounds still hold*!

Numerical experiments

Numerical experiments

- Given $0 < \lambda_1 < \lambda_n$: $A = \mathrm{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$,

$$\boxed{\lambda_i = \lambda_1 + \frac{i-1}{n-1}(\lambda_n - \lambda_1)\rho^{(n-i)}, \quad i = 2, \dots, n-1, \quad \rho \in [0,1].}$$

[1] We follow the settings described in (Carson, Liesen, and Strakoš 2024), and (Vieublé 2022) for these constructions.

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- For $j \in \{2, 3, \ldots, n\}$ we set $M = \mathrm{diag}(\lambda_1, \ldots, \lambda_{j-1}, \lambda_j, \ldots, \lambda_j)$, and let $M = LL^\top$[1].

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- In exact arithmetic, the matrices $M^{-1}A$, AM^{-1} and $L^{-1}AL^{-\top}$ are similar with the spectrum

$$S = \left\{1, \frac{\lambda_{j+1}}{\lambda_j}, \frac{\lambda_{j+2}}{\lambda_j}, \dots, \frac{\lambda_n}{\lambda_j}\right\},$$

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- We set $n = 85$, $b = \frac{1}{\sqrt{n}} \cdot [1, \ldots, 1]^\top$, $x_0 = [0, \ldots, 0]^\top$ for all the experiments.

- We also fix $\lambda_1 = 1, \lambda_n = 10^5$, and $\rho = 0.6 \implies$ accumulation of eigenvalues to the left.

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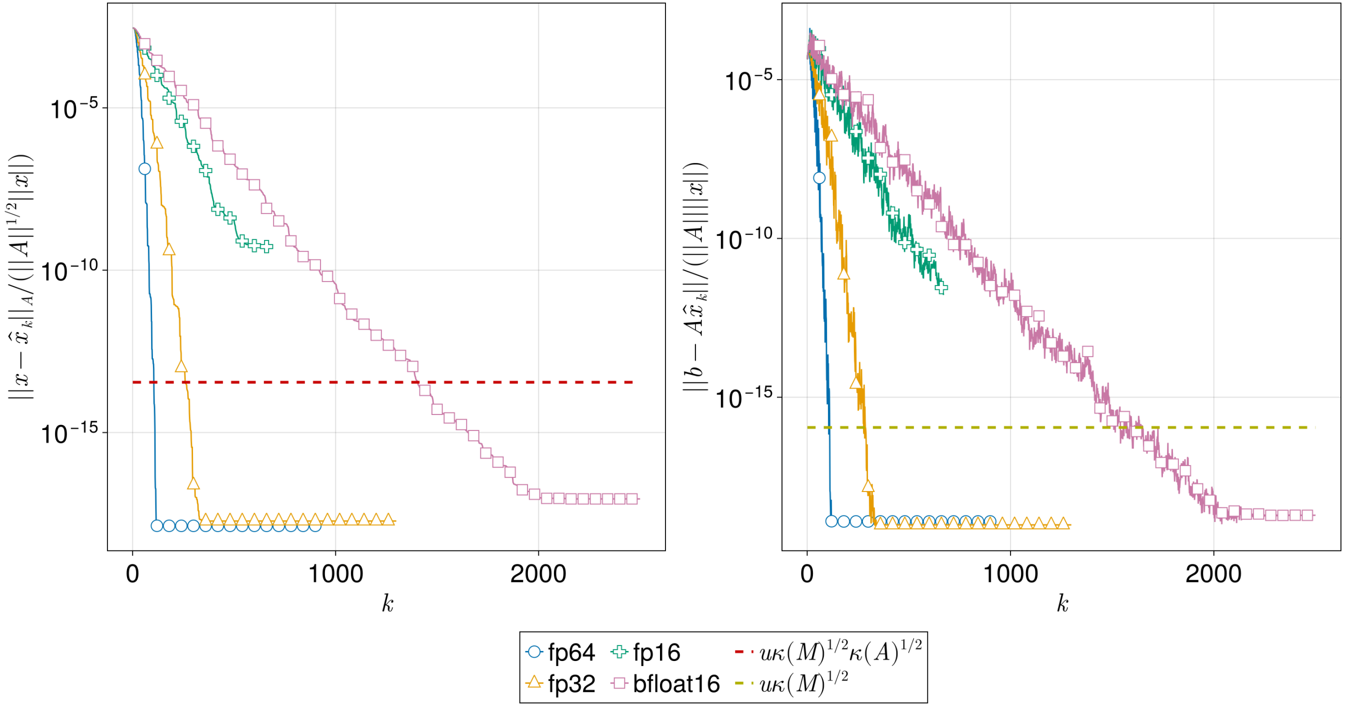
Left PCG

- Set $j = 55$



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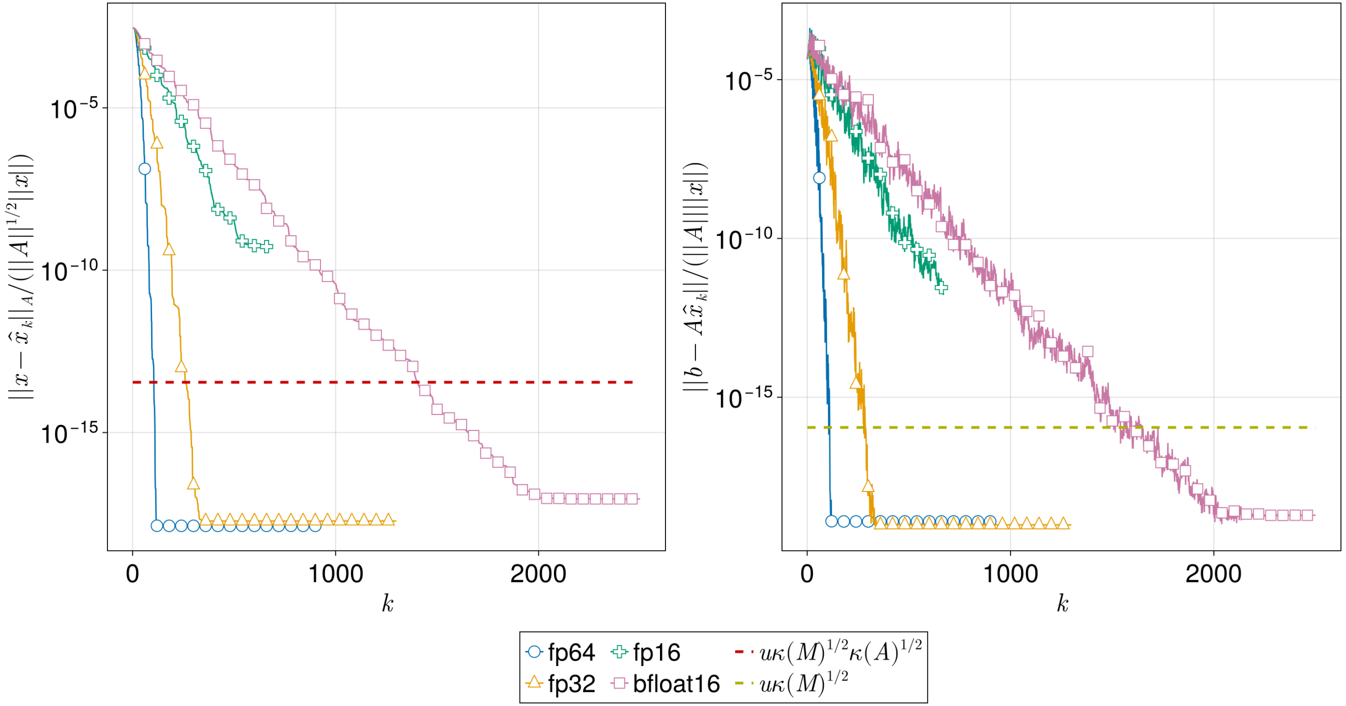

Arithmetic	Unit roundoff	Smallest subnormal number
bfloat16	3.91×10^{-3}	9.18×10^{-41}
fp16 (half)	4.88×10^{-4}	5.96×10^{-8}
fp32 (single)	5.96×10^{-8}	1.40×10^{-45}
fp64 (double)	1.11×10^{-16}	4.94×10^{-324}

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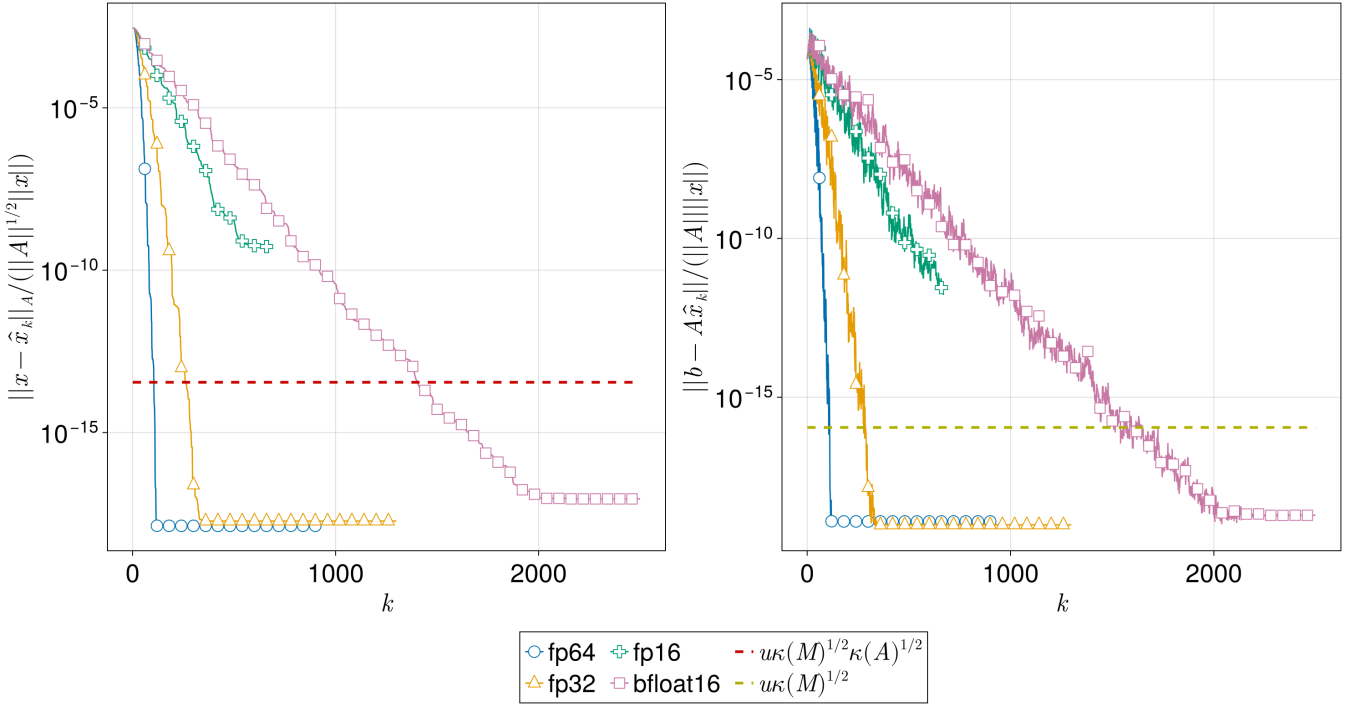

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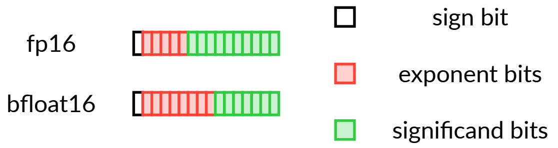
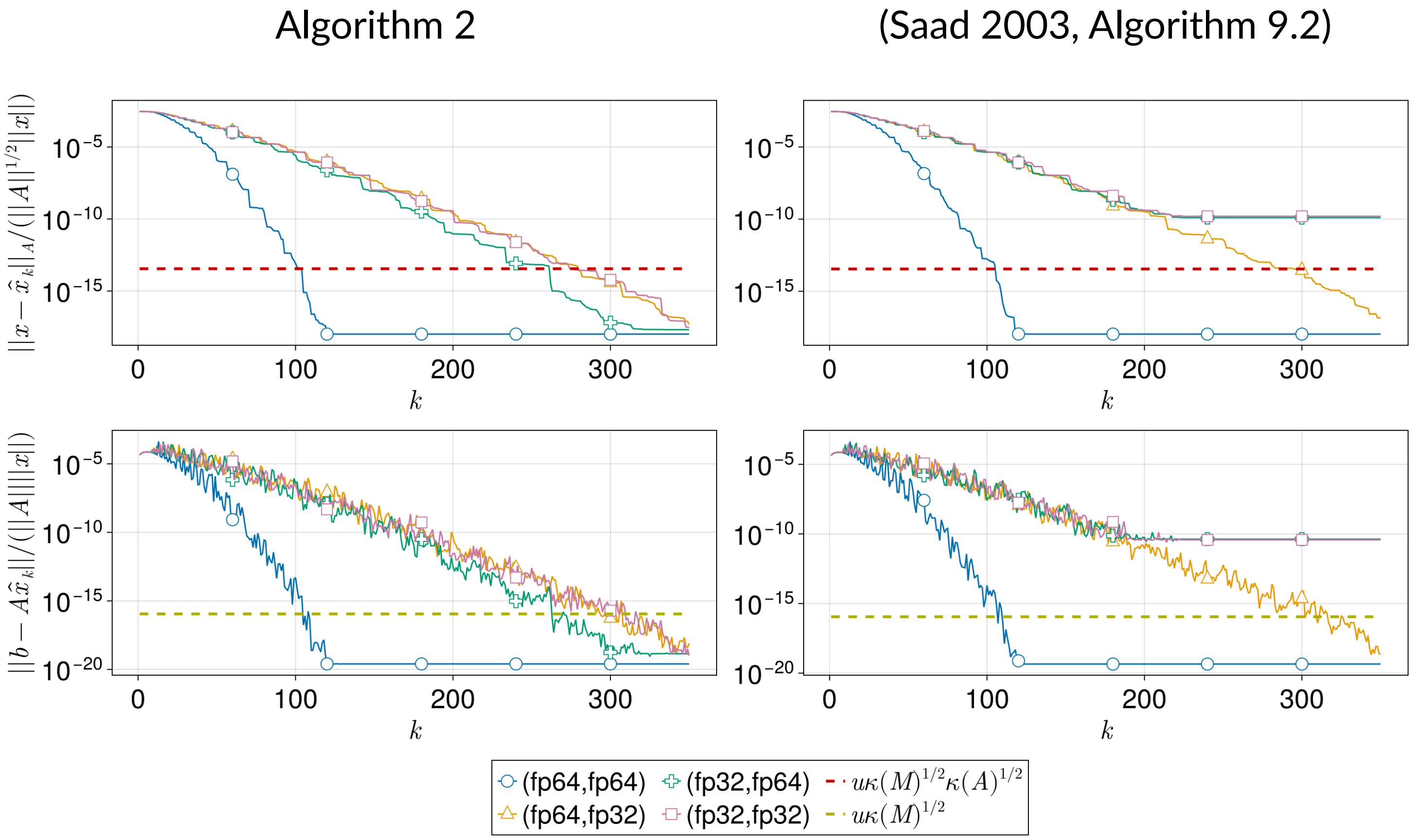


Split PCG comparison

- Set $j = 65$.



Split PCG comparison

Algorithm 2

$$r_{k+1} = r_k - \alpha_k A p_k$$

$$s_{k+1} = M_L^{-1} r_{k+1}$$

$$\|b - A\hat{x}_k - \hat{r}_k\| \le (nk\boldsymbol{u})\|A\| \max_{j\le k}\Big(\|\hat{x}_j\|, \|x\|\Big)$$

(Saad 2003, Algorithm 9.2)

$$r_{k+1} = r_k - \alpha_k M_L^{-1} A p_k$$

$$\|b - A\hat{x}_k - \hat{r}_k\| \le \|A\| \cdot \max_{j\le k}\Big(\|\hat{x}_j\|, \|x\|\Big)\Big[O(nk\boldsymbol{u}) + O(\boldsymbol{u}_s)\kappa(M_L)\Big]$$

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Thank you for your attention!

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