Residual Replacement in Mixed-Precision Iterative Refinement for Sparse Linear Systems

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Mixed Precision Iterative Refinement

- Given a linear system $A\hat{x} = \hat{b}$, *iterative refinement* (IR) is a technique to improve the accuracy of an initial solution $\hat{x}_0$:

$$
\begin{aligned}
&\textbf{for } k := 0, 1, 2, \ldots \\
&\qquad r := \hat{b} - A\hat{x}_k && \text{Residual calculation} \\
&\text{Solve } Ay = r \text{ for } y && \text{Inner solver} \\
&\qquad \hat{x}_{k+1} := \hat{x}_k + y && \text{Solution update}
\end{aligned}
$$

- Any inner solver: dense/sparse factorization…
  even an iterative Krylov(-type) solver
- In machine precision u, provided $uk(A) \leq 1$, IR eventually produces an accurate solution to full precision u

Mixed Precision Iterative Refinement

- On many architectures, IR can be efficiently combined with mixed precision (single-double, half-double, half-single)

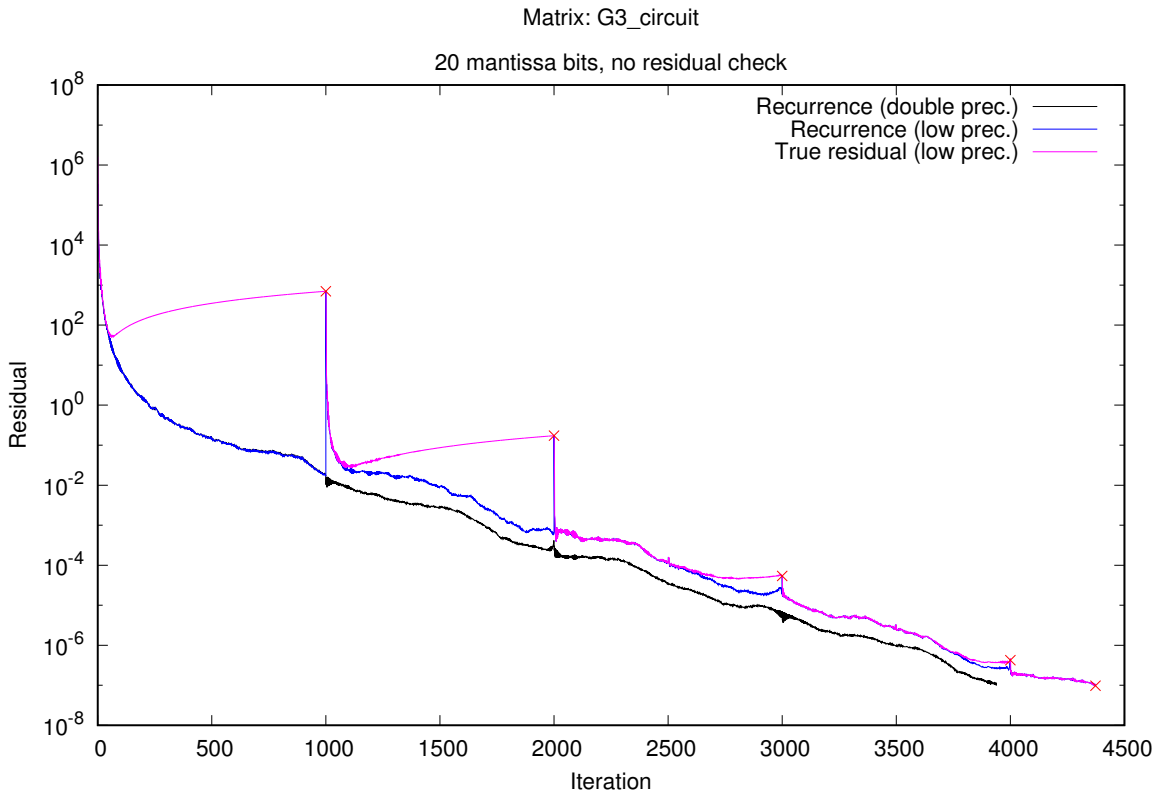
for $k := 0, 1, 2, \ldots$

$r := \hat{b} - A\hat{x}_k$	Residual calculation	Extended precision
Solve $Ay = r$ for y	Inner solver	Reduced precision
$\hat{x}_{k+1} := \hat{x}_k + y$	Solution update	Extended precision

- Most of the cost is in the inner solver
- Accuracy is improved by the outer refinement process

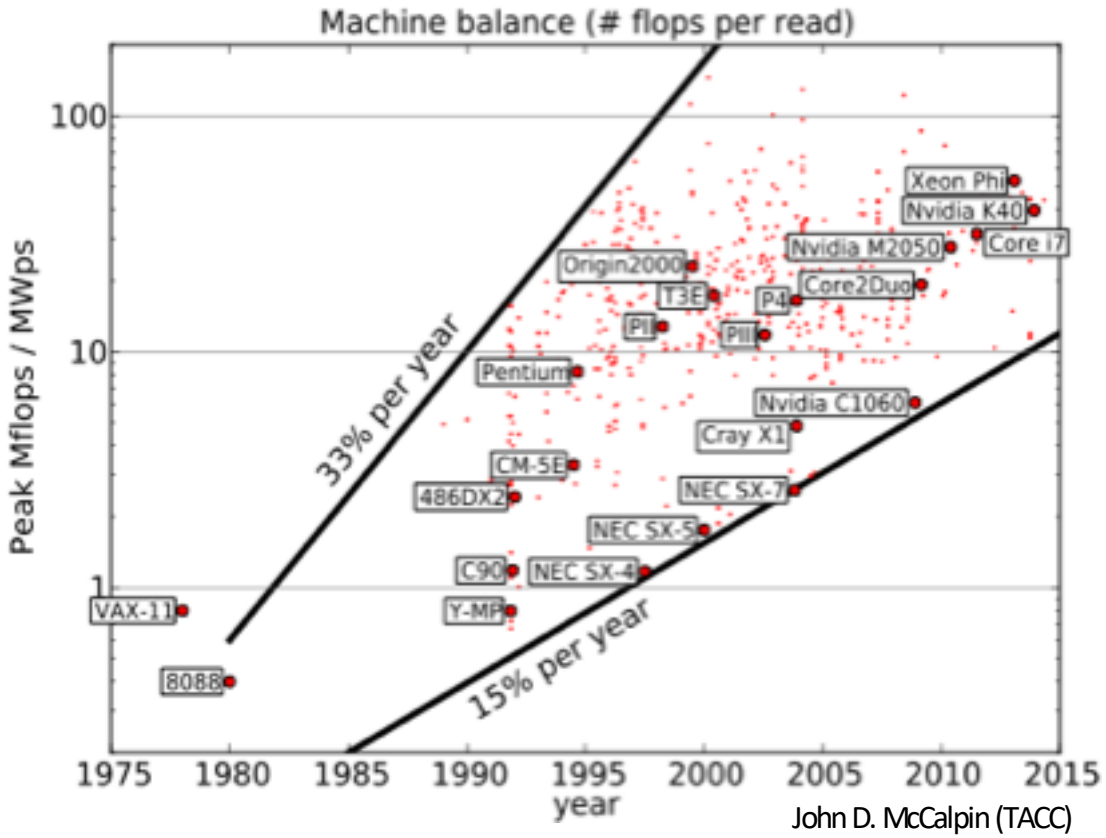
Mixed Precision Iterative Refinement

- Can MPIR be efficiently combined with an iterative Krylov inner solver?
  - Maintain **convergence rate** by avoiding numerical pitfalls in the recurrence residual due to finite precision



Mixed Precision Iterative Refinement

- What are the potential gains of mixed precision?
  - For Krylov solvers applied to sparse linear systems, **the theoretical cost/energy/time is in moving data, not in arithmetic**



John D. McCalpin (TACC)

Outine

- Residual replacement for Krylov solvers
- Cost model
- Explicit residual deviation with MPIR
- Cost evaluation
- Customized precision via mantissa segmentation

Residual Replacement for Krylov Solvers

- Preconditioned Conjugate Gradient (PCG)

$r_0 := b - Ax_0,\ z_0 := M^{-1}r_0,\ d_0 := z_0,\ \beta_0 := r_0^T z_0,$	Initializations
$\tau_0 :=\| r_0 \|_2,\ j := 0$	
while $(\tau_j > \tau_{\max})$	**Iterative PCG solve**
$w_j := Ad_j$	SPMV
$\rho_j := \beta_j / d_j^T w_j$	DOT product
$x_{j+1} := x_j + \rho_j d_j$	AXPY
$r_{j+1} := r_j - \rho_j w_j$	AXPY
$z_{j+1} := M^{-1} r_{j+1}$	Preconditioning
$\beta_{j+1} := r_{j+1}^T z_{j+1}$	DOT product
$\alpha_j := \beta_{j+1} / \beta_j$	
$d_{j+1} := z_{j+1} + \alpha_j d_j$	AXPY-like
$\tau_{j+1} :=\| r_{j+1} \|_2$	2-norm
$j := j + 1$	
endwhile	

Residual Replacement for Krylov Solvers

- Preconditioned Conjugate Gradient (PCG)

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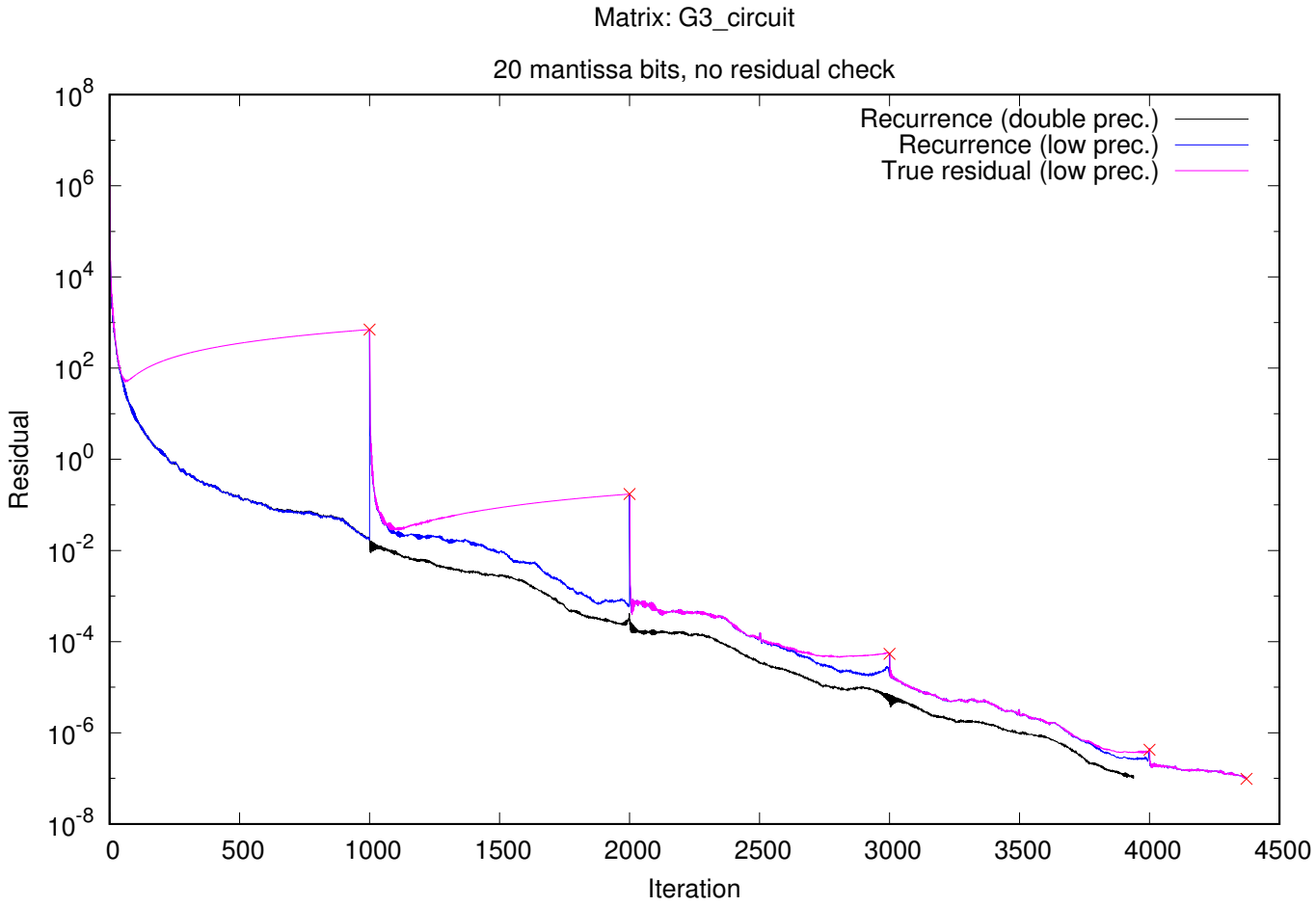
True residual

$$b - Ax_{j+1}$$

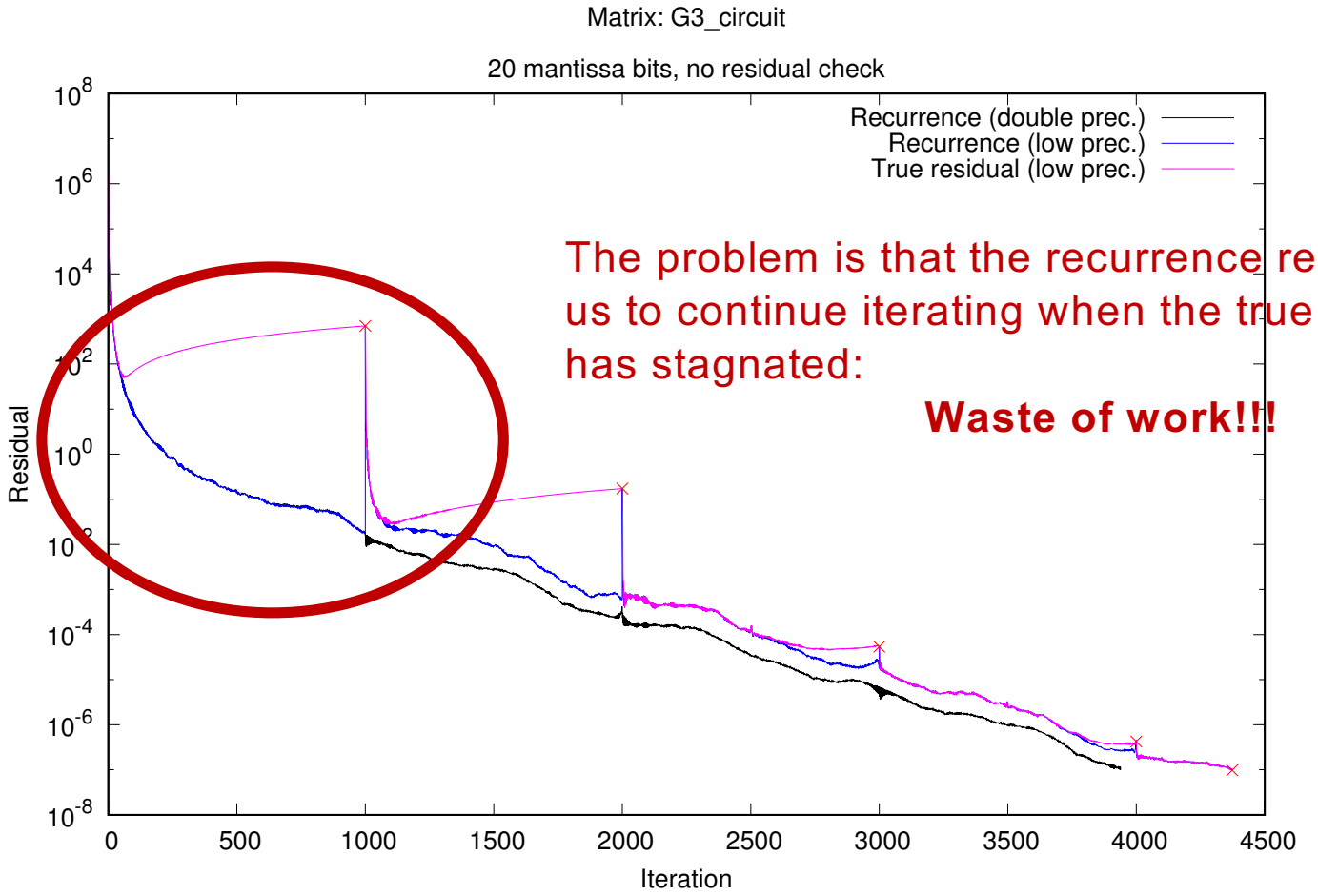
Residual Replacement for Krylov Solvers

- Divergence between **recurrence** vs **true** residuals



Residual Replacement for Krylov Solvers

- Finite precision causes divergence between recurrence vs true residuals



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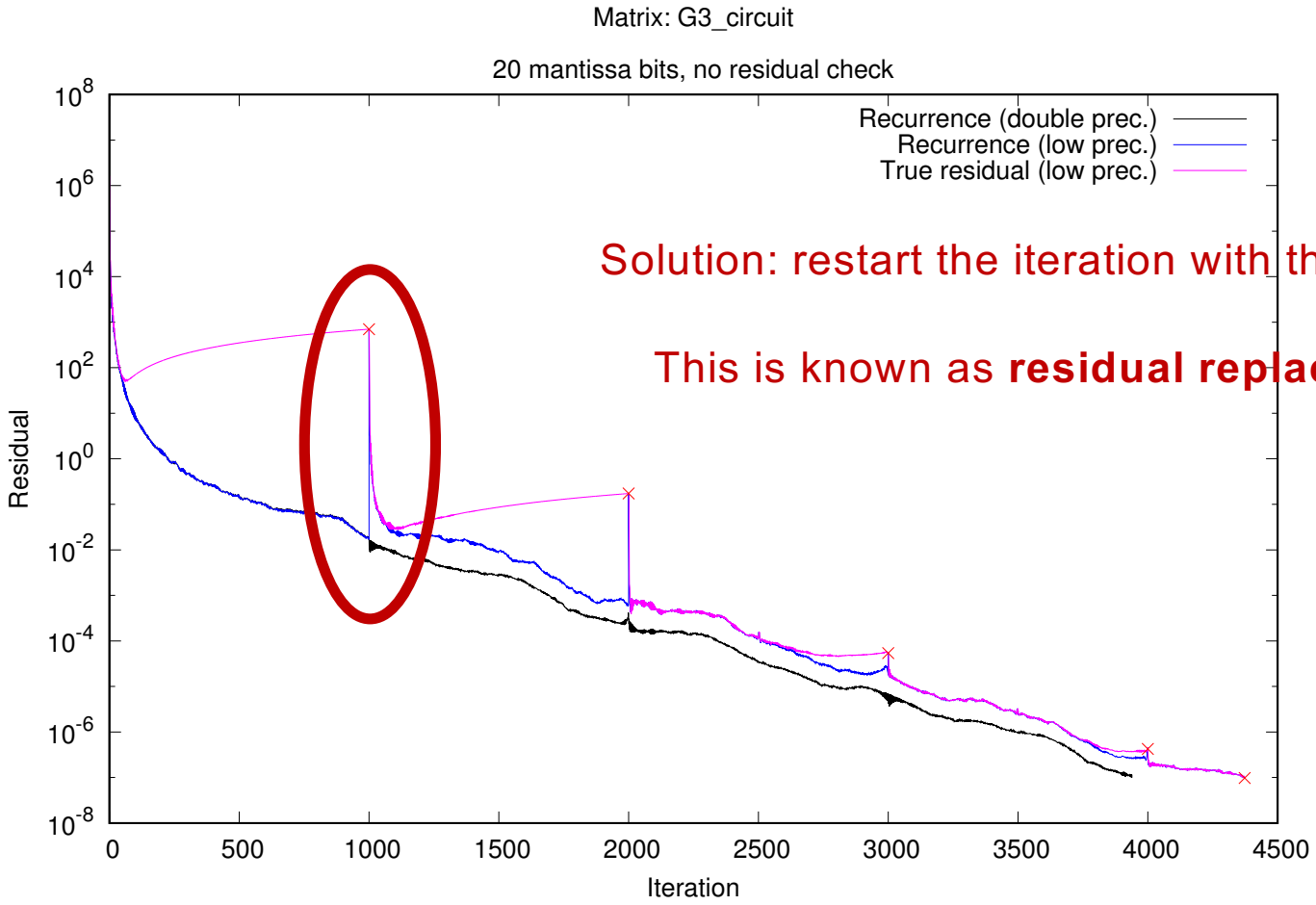

Solution: restart the iteration with the true residual

This is known as **residual replacement (RR)**

Residual Replacement for Krylov Solvers

- Divergence problem can be tackled via RR:
  - **Replace always** (at every iteration): 2 SpMV per iteration and may deteriorate the convergence of the iteration
  - **Replace periodically** (every t iterations): may deteriorate the convergence of the iteration
  - **Compute explicit deviation at every iteration and replace if needed:** 2 SpMV per iteration
  - **Estimate deviation and replace if needed:**

H. A. Van der Vorst, Q. Ye. "Residual replacement strategies for Krylov subspace iterative methods for the convergence of true residuals." SIAM J. Sci. Comput., 22(3), 2000

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- **Van der Vorst and Ye** (VY), 2000. Keep track of accumulated deviation:

$$d_0 = d_{init} := u_r(||r_0|| + N||A||||x_0||),$$
$$d_{j+1} := d_j + u_r(||r_j|| + N||A||||\tilde{x}_j||), \quad j = 0, 1, 2, \ldots,$$

Then, perform RR if the following three conditions hold

$$d_j \leq \epsilon||r_j||, \qquad d_{j+1} > \epsilon||r_{j+1}||, \qquad d_{j+1} \geq 1.1\, d_{init}$$

- Compared with others, VY's RR technique:
  - Aims for small deviations between recurrence/true residuals
  - Preserves convergence mechanism of the iteration
  - It is cheap and easy to add to existing Krylov implementations

Residual Replacement for Krylov Solvers

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- Experiments proving effectiveness of VY's RR technique:
  - 28 matrices for Harwell-Boeing collection, BiCG and CGS methods
  - Only double precision arithmetic
  - #iterations not reported, only #RR
  - Convergence threshold set close to machine precision (likely impractical)

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  - Only double precision arithmetic
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- Differences:
  - CG method
  - Integration in an outer-inner scheme for iterative refinement: MPIR
  - #iterations is important!
  - Convergence to more realistic residual bounds
  - Cost model

Cost Model

- Premises:
  - For a memory-bound algorithm, such as PCG applied to a sparse linear system, the “cost” is dominated by data movement while floating-point arithmetic is irrelevant
    - If cost = execution time, arithmetic cost is minor (memory wall) and can be overlapped with communication
    - If cost = energy, accesses to main memory are much more expensive than arithmetic

Operation	approximate energy cost
DP floating point multiply-add	100 pJ
DP DRAM read-to-register	4800 pJ

Cost Model

- Premises (cont'd):
  - After each particular operation, data does not remain in cache (large vectors)
  - Costs are linearly dependent on the bit-length of data
  - Problem of size n, with sparse matrix stored in CSR format consisting of n_z nonzero entries
  - Simple Jacobi preconditioner for CG

Cost Model

- SpMV, in CSR format, using data with xx bits in terms of bit transfers (or cost-units, cus):

```
y = A * x;
    CSR A:  row_ptr[n],
            col_idx[nz],
            val[nz]
```

```
for (i=0; i<n; i++) {
  tmp = 0;
  for (j=row_ptr[i]; j<row_ptr[i+1]; j++)
    tmp += val[j] * x[col_idx[j]];
  y[i] = tmp;
}
```

$$\mathcal{C}_{\mathrm{SPMV}}(\mathrm{xx}) = \underbrace{(n + 2n_z) \cdot \mathsf{fpxx}}_{\text{Vector, matrix entries}} + \underbrace{(n + n_z) \cdot \mathsf{int32}}_{\text{indices}} \quad \mathrm{cus}$$

Cost Model

- PCG solver operating with xx bits:

$r_0 := b - Ax_0,\ z_0 := M^{-1}r_0,\ d_0 := z_0,\ \beta_0 := r_0^T z_0,$	Initializations
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$$\mathcal{C}_{\text{PCG}}^{\text{iter}}(\text{xx}) = \underbrace{14n \cdot \text{fpxx}}_{\text{vector ops.}} + \mathcal{C}_{\text{SPMV}}(\text{xx}) + \underbrace{3n \cdot \text{fpxx}}_{\text{preconditioner appl.}} \quad \text{cus}$$

Cost Model

- For MPIR-VY, cost depends on:
  - #IS: number of iterations of inner solver
  - #RR: total number of residual replacements
  - #RS: number of refinement steps
- For example, using (32,64) mixed precision:

$$\mathcal{C}^{\mathrm{VY}}_{\mathrm{MPIR}}(32{,}64) = \underbrace{\mathcal{C}^{\mathrm{iter}}_{\mathrm{PCG}}(32) \cdot \#\mathrm{IS}}_{\text{Plain inner PCG solver}} + \underbrace{n \cdot \mathsf{fp32} \cdot \#\mathrm{IS}}_{\text{Replacement condition test}}$$
$$+ \underbrace{(4n \cdot \mathsf{fp32} + \mathcal{C}_{\mathrm{SPMV}}(32)) \cdot \#\mathrm{RR}}_{\text{RRs in inner PCG solver}}$$
$$+ \underbrace{(6n \cdot \mathsf{fp64} + n \cdot \mathsf{fp32} + \mathcal{C}_{\mathrm{SPMV}}(64)) \cdot \#\mathrm{RS}}_{\text{Refinement steps}} \quad \text{cus}$$

Explicit Residual Deviation with MPIR

- Our RR technique: **Explicit residual deviation** (ERD)
  - Test periodically (i.e., every t iterations)

$$\|r_{k+1}^{true}\|_2 / \|r_{k+1}^{rec}\|_2 \geq \tau$$

Computing the residual explicitly is expensive (SpMV), but it can be done **in reduced precision**

Cost can be further reduced by performing the residual calculation together with SpMV for inner solver

  - If deviation exceeds the threshold, stop the inner solver and start a new iteration of refinement (outer level) → enforces a residual replacement **in extended precision**

Explicit Residual Deviation with MPIR

- Cost of ERD-RR:

$$\mathcal{C}^{\text{ERD}}_{\text{MPIR}}(32,64) = \underbrace{\mathcal{C}^{\text{iter}}_{\text{PCG}}(32) \cdot \#\text{IS}}_{\text{Plain inner PCG solver}} + \underbrace{(4n \cdot \text{fp32} + \mathcal{C}_{\text{SPMV}}(32)) \cdot \#\text{IS}/t}_{\text{Residual tests in inner PCG solver}} + \underbrace{(6n \cdot \text{fp64} + n \cdot \text{fp32} + \mathcal{C}_{\text{SPMV}}(64)) \cdot \#\text{RS}}_{\text{Refinement steps}} \quad \text{cus}$$

Explicit Residual Deviation with MPIR

- VY vs EDR:
  - VY-RR incurs detection overhead at each iteration (test replacement condition) and pays correction overhead in case RR is necessary
  - EDR-RR incurs detection overhead only every t iterations (periodicity of the test), risking to waste work in case of stagnation from last test
  - Detection techniques are different and, therefore, also are numerical effects and overhead:

Apply RR in the inner solver, and continue with iteration

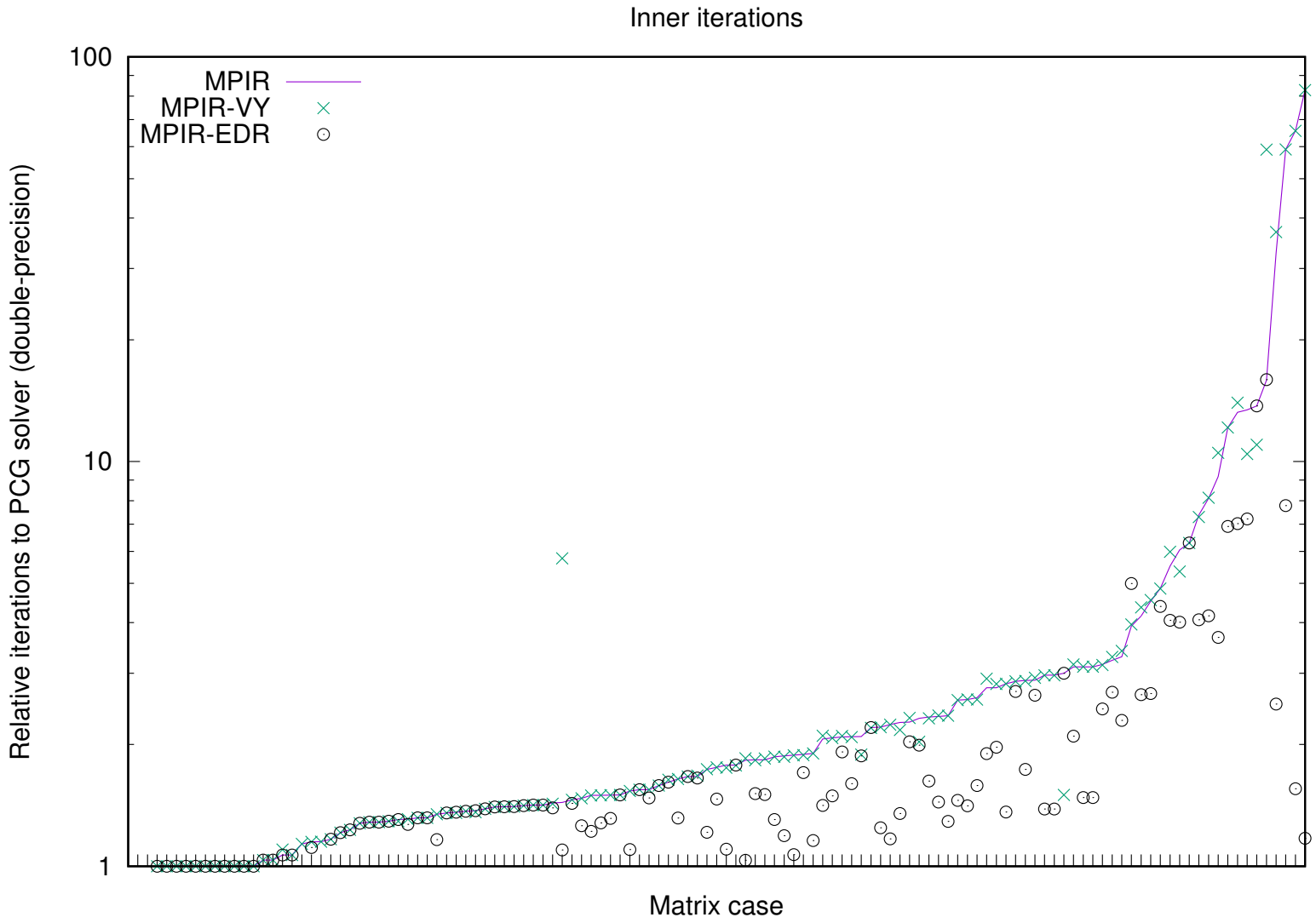
vs

Apply RR by ”moving” to the outer solver

Cost Evaluation

- Setup:
  - 123 symmetric positive definite matrices from SuiteSparse Matrix Collection (formerly UFMC)
  - Baseline solver: PCG in double precision
  - All arithmetic done in double precision
  - For MPIR variants, all data used in the inner solver are stored in single precision: **reduced transfer cost!**
  - For EDR-RR, the test is performed every t = 100 iterations, and the maximum number of RR is set to 10
  - Cost take into account the actual number of iterations to obtain an absolute residual error below 10^{-7}

Cost Evaluation



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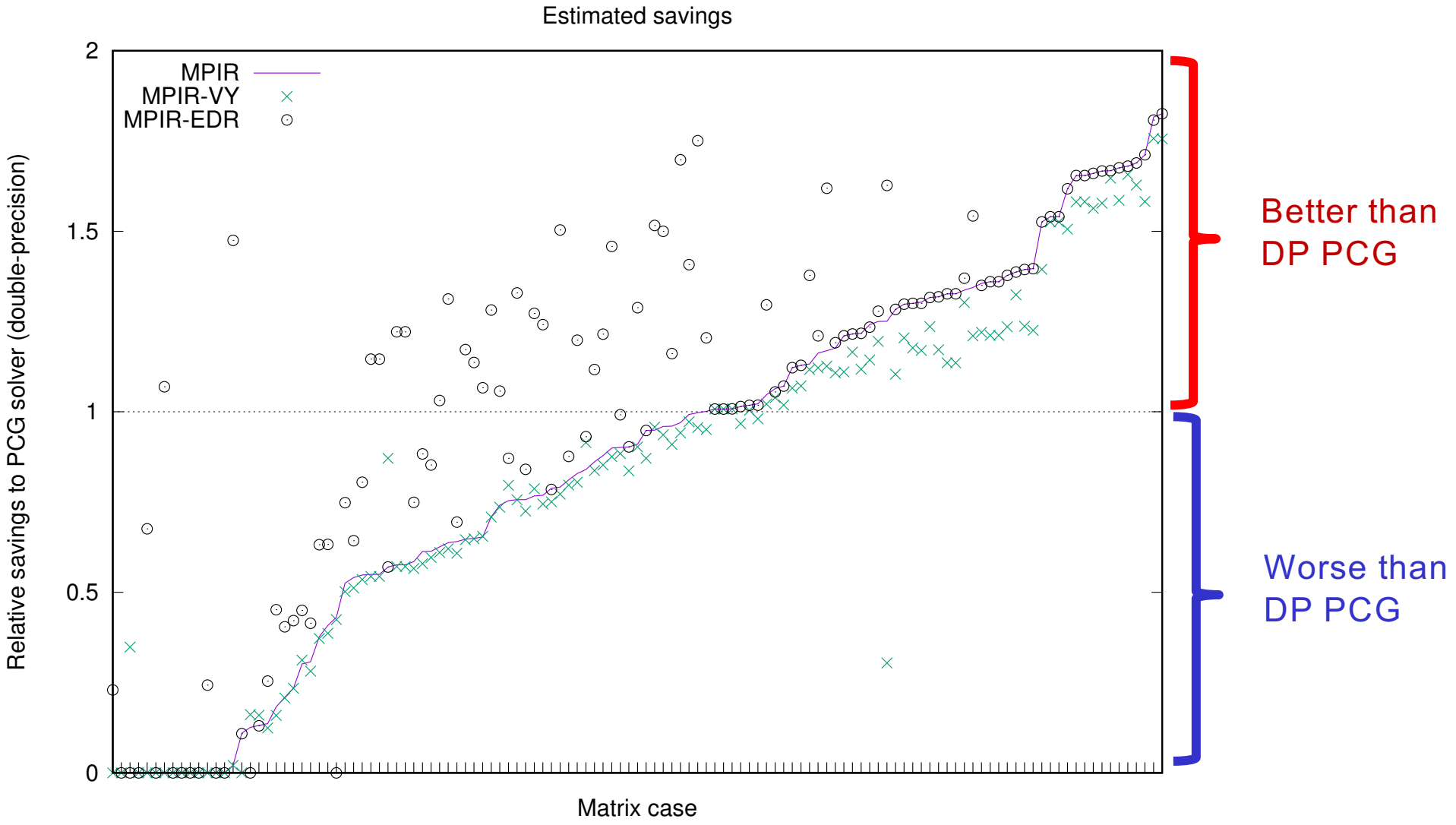


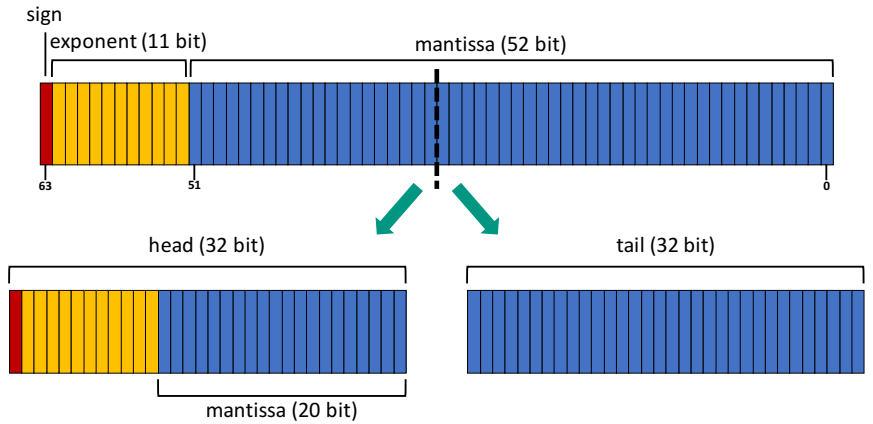
Customized Precision via Segmentation

- Decouple arithmetic from storage formats:
  - FPUs only support a limited number of IEEE 754 formats (single, double and, in some architectures, half)
  - … but we are free to store the data in memory in any **customized format**
- Remember: As a memory-bound algorithm, PCG is limited by memory bandwidth (i.e., how many bit are used to store the data)
  - Extended can be double
  - Reduced can be, e.g., 16, 24, 32, 40, 48, 56 bits
  - Maintain a single copy of the matrix with “multiple precisions” via **segments**

T. Grützmacher, H:. Anzt. “A modular precision format for decoupling arithmetic format and storage format”. Submitted to HeteroPar 2018

Customized Precision via Segmentation

- Split the IEEE double precision format into segments.
  (2-segment modular precision, 4-segment modular precision…)



- *Special "conversion" routines to double precision.*
- *Mantissa much shorter than IEEE single/half precision.*
- *No under- / overflow.*

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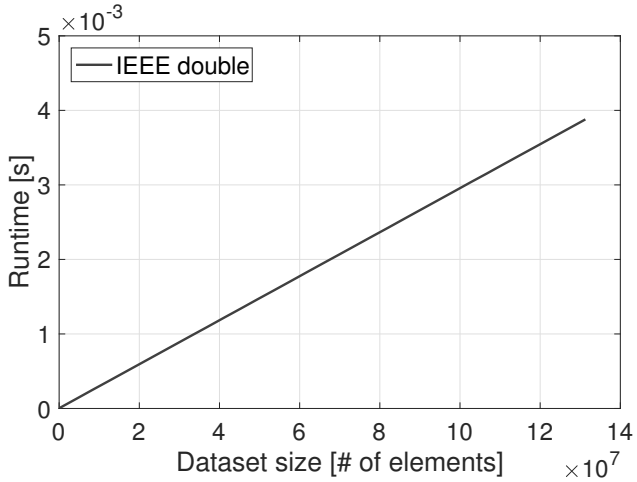

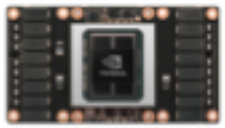

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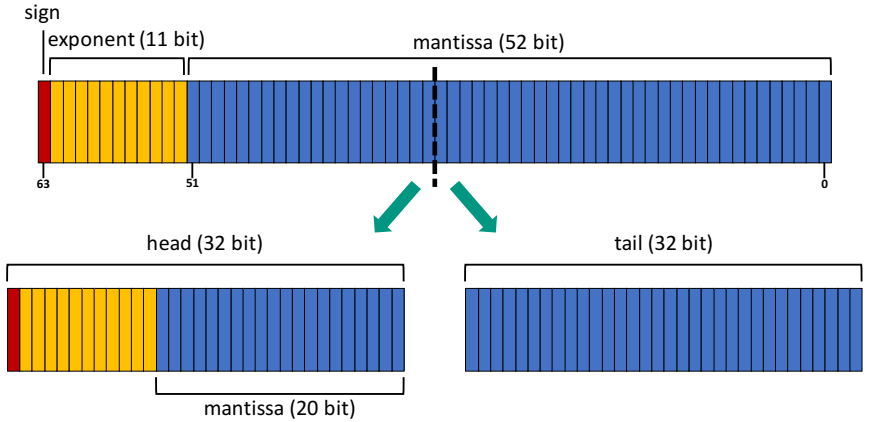

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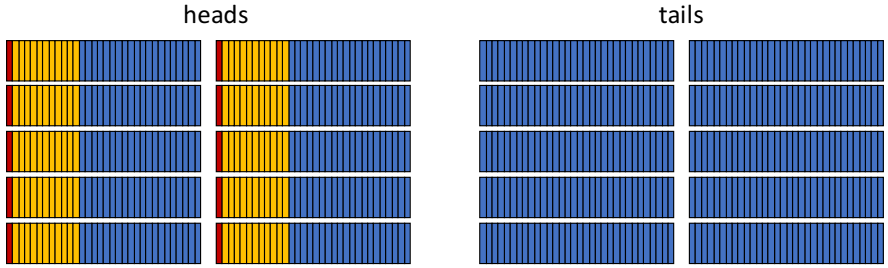

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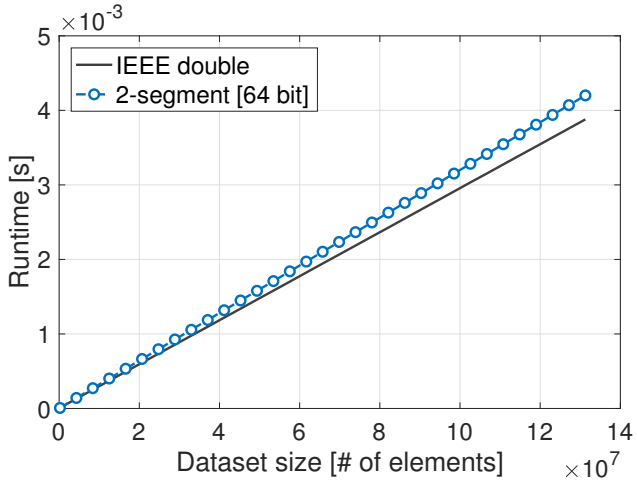

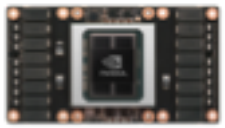

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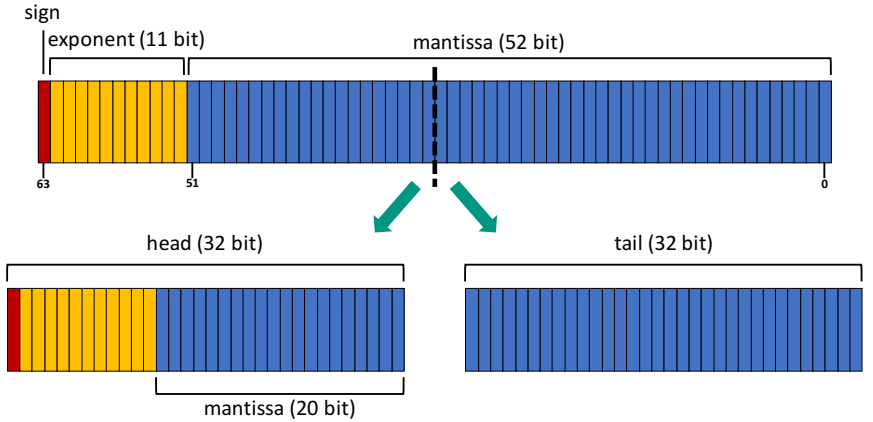

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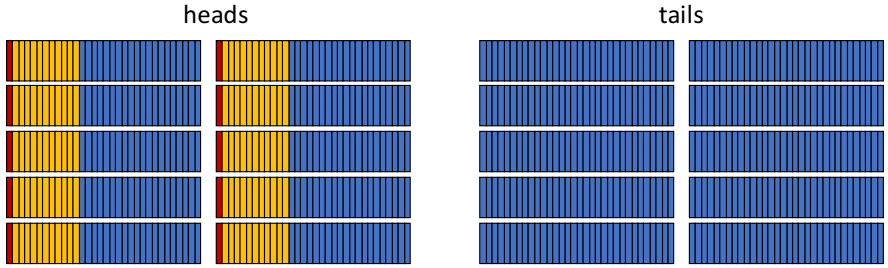

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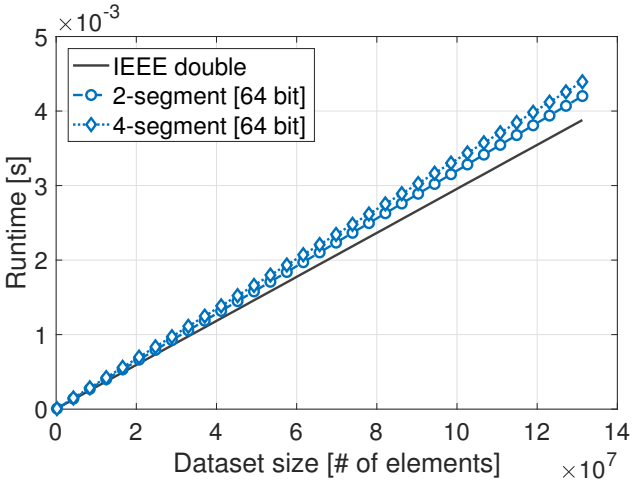

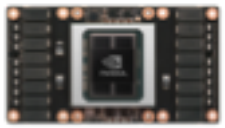

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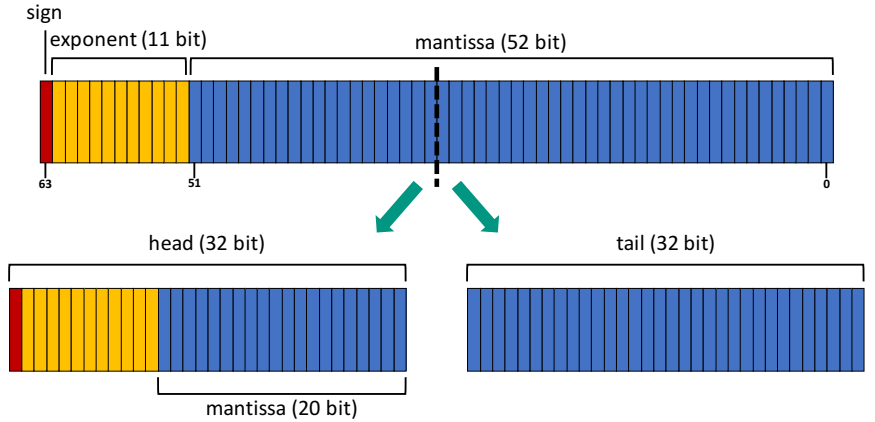

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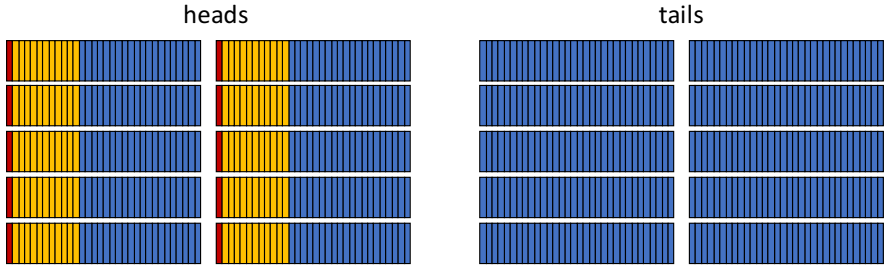

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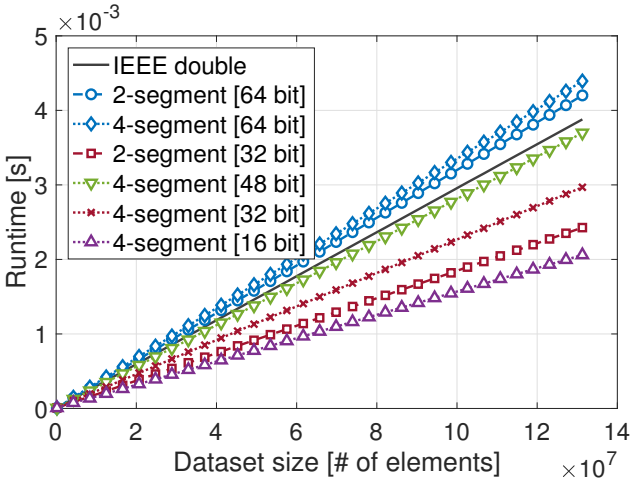

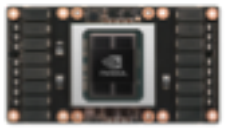

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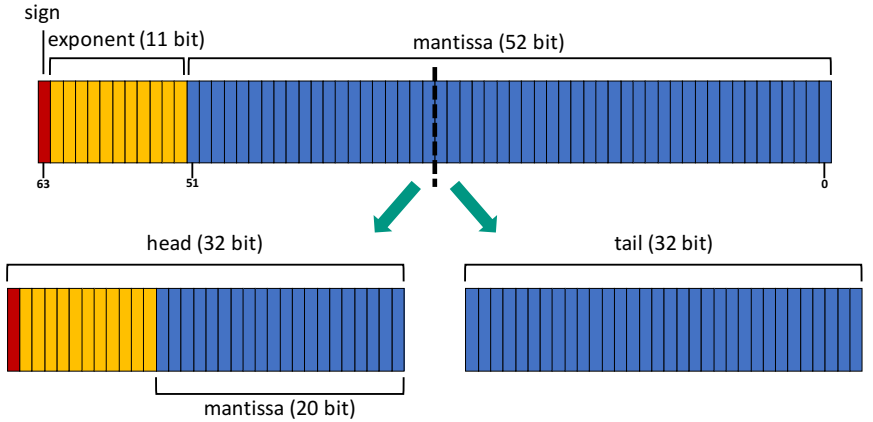

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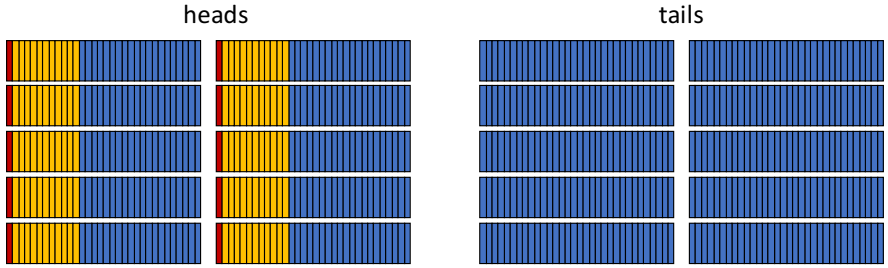

Concluding Remarks

- MPIR can be efficiently combined with any inner Krylov solver provided it is enhanced with an appropriate RR technique
- Theoretical savings can be significant in terms of reduced memory bandwidth: lower energy and computational costs
- Reduced precision storage in the inner solver can be realized via modular precision formats