The Multiprecision Effort in the US Exascale Computing Project

ICERM: Variable Precision in Mathematical and Scientific Computing

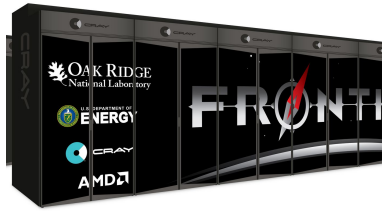
May 7th / May 8th 2020

Hartwig Anzt & FiNE@KIT in collaboration with Jack Dongarra & ICL, Ulrike Meier Yang, Enrique Quintana-Orti, and many others...

What is the Multiprecision Effort in ECP

- Coordinated effort across all math library projects of the US Exascale Computing Project;
- Administratively part of the xSDK4ECP project led by Ulrike Meier Yang;
- Link between multiprecision efforts of ECP project partners and create synergies across the individual efforts;
- Evaluate status quo and develop and deploy production-ready software;
- Algorithm focus on linear solvers, eigenvalue solvers, preconditioners, multigrid methods, FFT, Machine Learning (ML) technology;
- Hardware focus on leadership computers (Summit, Frontier…);
- We are focusing on performance, not (bit-wise) reproducibility;

Ulrike Meier Yang (LLNL)

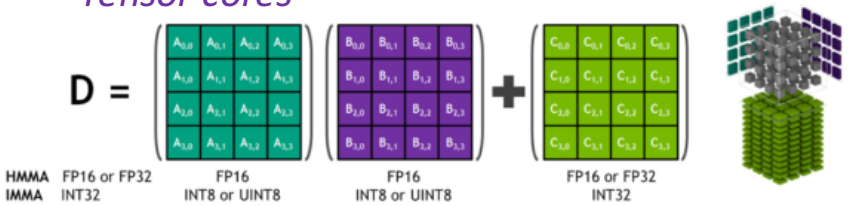


Floating point formats and performance on GPUs

	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020
NVIDIA GPU generation			Tesla		Fermi			Kepler		Maxwell		Pascal		Volta	
Rel. compute performance			1 : 8		1 : 8			1 : 24		1 : 32		1 : 2 : 4		1 : 2 : 16*	
Rel. memory performance			1 : 2		1 : 2			1 : 2		1 : 2		1 : 2 : 4		1 : 2 : 4	

double : single : half

*Tensor cores



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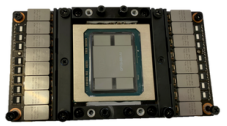
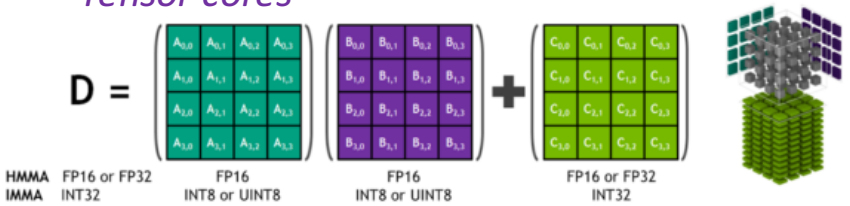


double : single : half

For compute-bound applications, the performance gains from using lower precision depend on the architecture.

Up to 16x for FP16 on Volta, up to 32x for FP32 on Maxwell.

**Tensor cores*



For memory-bound applications, the performance gains from using lower precision are architecture-independent and correspond to the floating point format complexity (#bits).

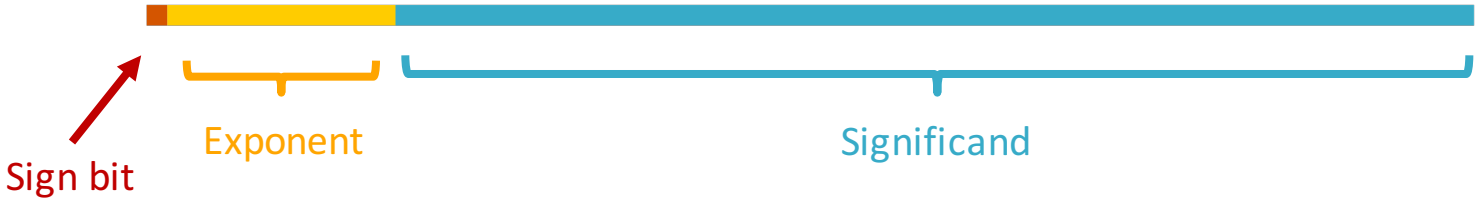
Generally, 2x for FP32, 4x for FP16.

Take-Away

- Performance of **compute-bound** algorithms depends on **format support of hardware**.
- Performance of **memory-bound** algorithms scales hardware-independent with **inverse of format complexity**.

Experiments based on the Ginkgo library https://ginkgo-project.github.io/ginkgo/examples/adaptiveprecision-blockjacobi/adaptiveprecision-blockjacobi.cpp

IEEE 754 Floating Point Formats



Broadly speaking….

- The length of the **exponent** determines the **range** of the values that can be represented;
- The length of the **significand** determines how **accurate** values can be represented;

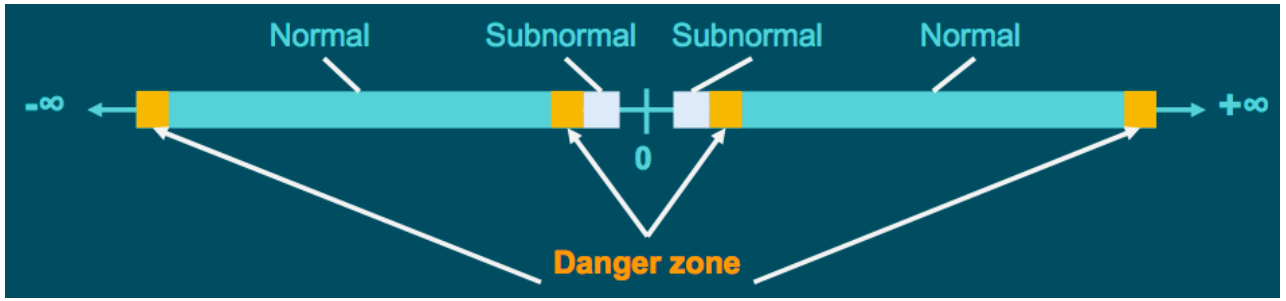
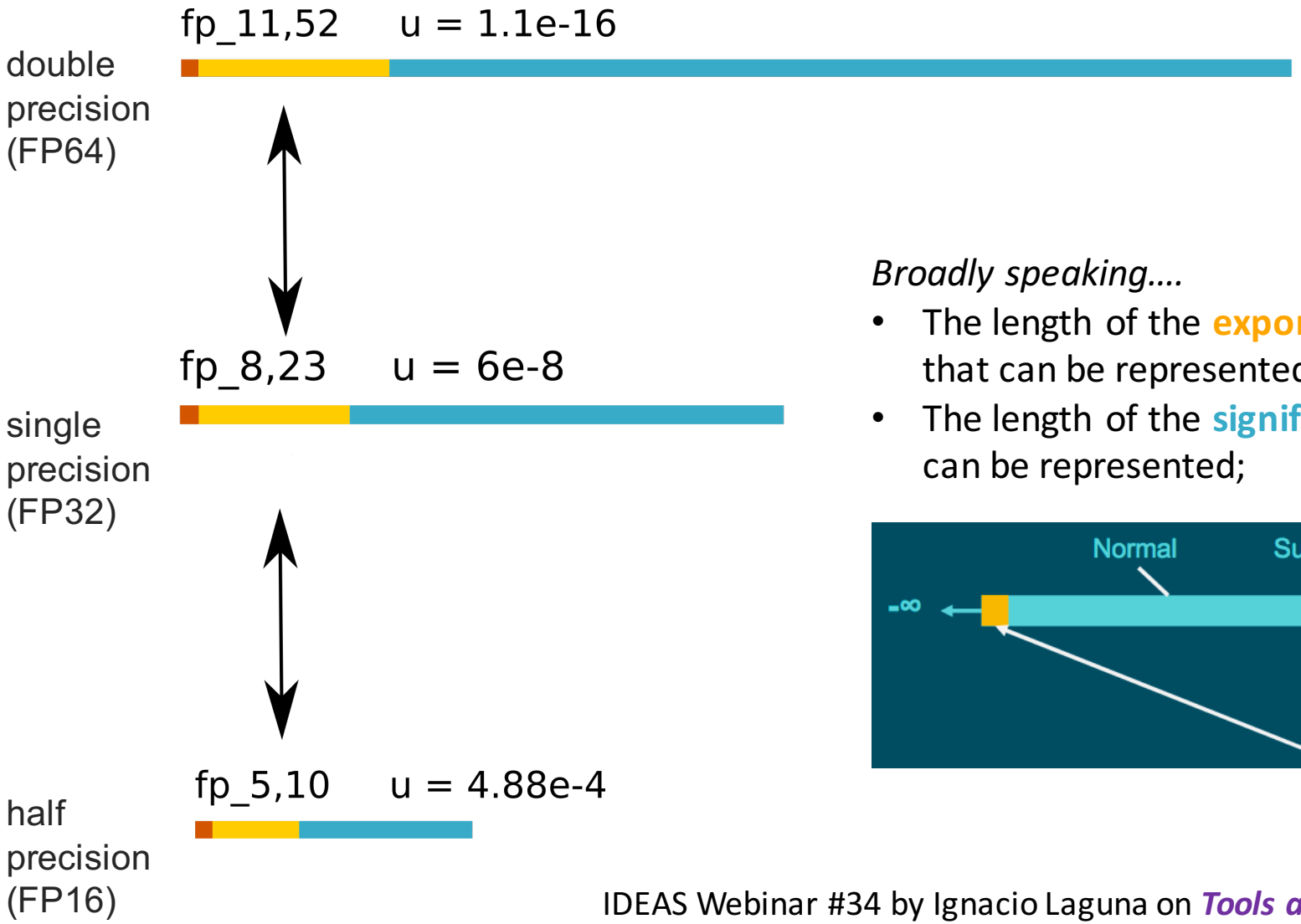


Figure courtesy of Ignacio Laguna, LLNL

IDEAS Webinar #34 by Ignacio Laguna on ***Tools and Techniques for Floating-Point Analysis***

IEEE 754 Floating Point Formats



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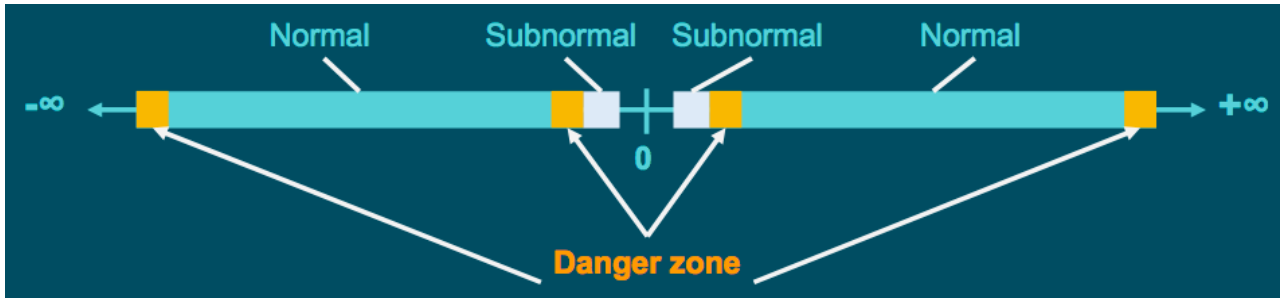

Figure courtesy of Ignacio Laguna, LLNL

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Floating point formats and accuracy

- The length of the **exponent** determines the **range** of the values that can be represented;
- The length of the **significand** determines how **accurate** values can be represented;

- *Rounding effects accumulate over a sequence of computations;*

Let us focus on linear systems of the form Ax=b.

- The conditioning of a linear system reflects how sensitive the solution x is with regard to changes in the right-hand side b.

- Rule of thumb:

relative residual accuracy = **(unit round-off)** * **(linear system's condition number)**

N. Higham: Accuracy and stability of numerical algorithms. SIAM, 2002.

Floating point formats and accuracy

Linear System Ax=b with cond(A) $\approx 10^4$

Experiments based on the Ginkgo library https://ginkgo-project.github.io/ginkgo/examples/adaptiveprecision-blockjacobi/adaptiveprecision-blockjacobi.cpp

Floating point formats and accuracy

Linear System Ax=b with cond(A) ≈ 10^4

Double Precision

```
Initial residual norm sqrt(r^T r):
%%MatrixMarket matrix array real g
1 1
111.127
Final residual norm sqrt(r^T r):
%%MatrixMarket matrix array real general
1 1
5.0775e-10
CG iteration count:     1231
CG execution time [ms]: 140.038
```

Accuracy improvement ~10^{12}

```
...
- ValueType = double;
+ ValueType = float;
...
```

relative residual accuracy = (unit round-off) * (linear system's condition number)

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Single Precision

```
Initial residual norm sqrt(r^T r):
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1 1
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Final residual norm sqrt(r^T r):
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1 1
0.179829
CG iteration count:     1234
CG execution time [ms]: 127.152
```

Accuracy improvement ~10^4

relative residual accuracy = (unit round-off) * (linear system's condition number)

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Floating point formats and accuracy

Linear System Ax=b with

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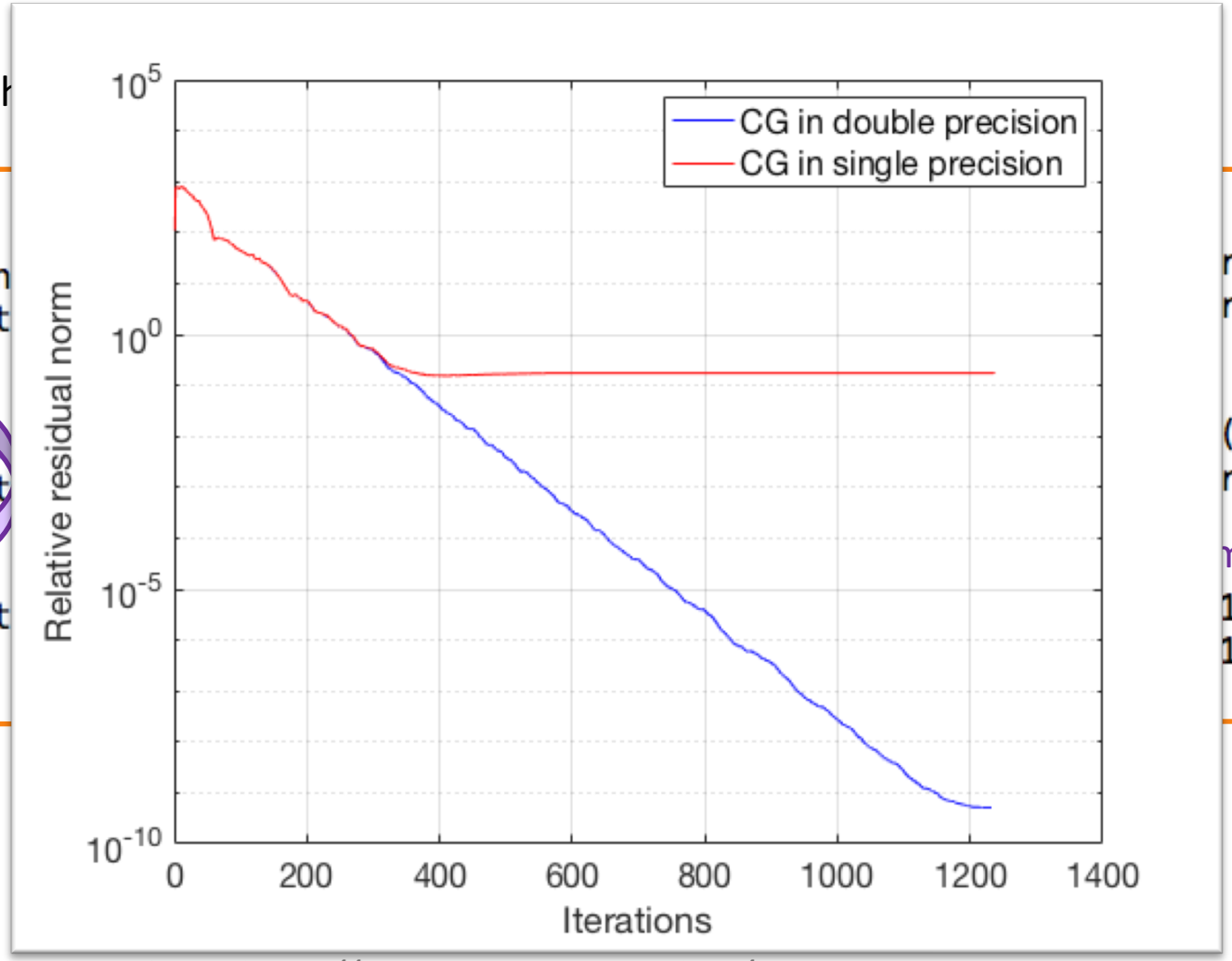


```
rt(r^T r):
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Single Precision is 10% faster!

Experiments based on the Ginkgo library https://ginkgo-project.github.io/ginkgo/examples/adaptiveprecision-blockjacobi/adaptiveprecision-blockjacobi.cpp

Floating point formats and accuracy

Linear System Ax=b with cond(A) ≈ 10^7

apache2 from SuiteSparse

Double Precision

```
Initial residual norm sqrt(r^T r):
%%MatrixMarket matrix array real general
1 1
1390.67
Final residual norm sqrt(r^T r):
%%MatrixMarket matrix array real general
1 1
4.53915e-06
CG iteration count:     6460
CG execution time [ms]: 2992.91
```

Accuracy improvement ~10^9

Single Precision

```
Initial residual norm sqrt(r^T r):
%%MatrixMarket matrix array real general
1 1
1390.67
Final residual norm sqrt(r^T r):
%%MatrixMarket matrix array real general
1 1
1588.77
CG iteration count:     8887
CG execution time [ms]: 2972.46
```

No improvement

Experiments based on the Ginkgo library https://ginkgo-project.github.io/ginkgo/examples/adaptiveprecision-blockjacobi/adaptiveprecision-blockjacobi.cpp

Take-Away

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- Performance of **memory-bound** algorithms scales hardware-independent with **inverse of format complexity**.
- **relative residual accuracy** = **(unit round-off)** * **(linear system's condition number)**
- If the problem is **well-conditioned**, and a **low-accuracy solution is acceptable**, use a **low precision format**. (i.e. IEEE single precision, or even IEEE half precision.)

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Framework for exploring the effect of floating point format in iterative solvers:

Ginkgo

https://github.com/ginkgo-project/ginkgo


Terry Cojean


Goran Flegar


Fritz Göbel


Thomas Grützmacher


Pratik Nayak


Tobias Ribizel


Mike Tsai

Low precision for solving ill-conditioned problems

- **Preconditioning iterative solvers.**
  - Idea: Approximate inverse of system matrix to make the system "easier to solve": $P^{-1} \approx A^{-1}$

    and solve $Ax = b \quad \Leftrightarrow \quad P^{-1}Ax = P^{-1}b \quad \Leftrightarrow \quad \tilde{A}x = \tilde{b}$.

Low precision for solving ill-conditioned problems

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- **Why should we store the preconditioner matrix P^{-1} in full (high) precision?**

Low precision for solving ill-conditioned problems

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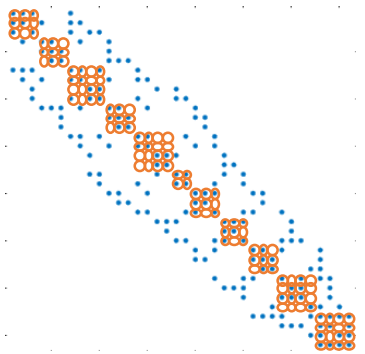
- **Why should we store the preconditioner matrix P^{-1} in full (high) precision?**

- **Jacobi method** based on **diagonal scaling** $P = diag(A)$
- **Block-Jacobi** is based on **block-diagonal scaling**: $P = diag_B(A)$
  - Each block corresponds to one (small) linear system.
    - *Larger* blocks typically improve convergence.
    - *Larger* blocks make block-Jacobi more expensive.



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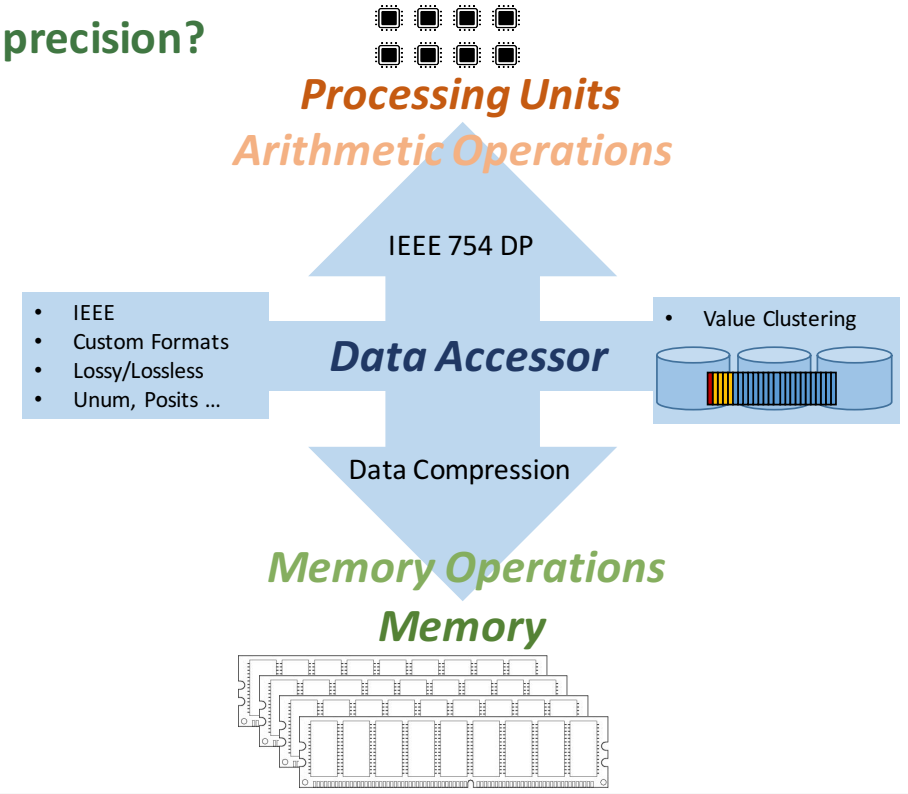
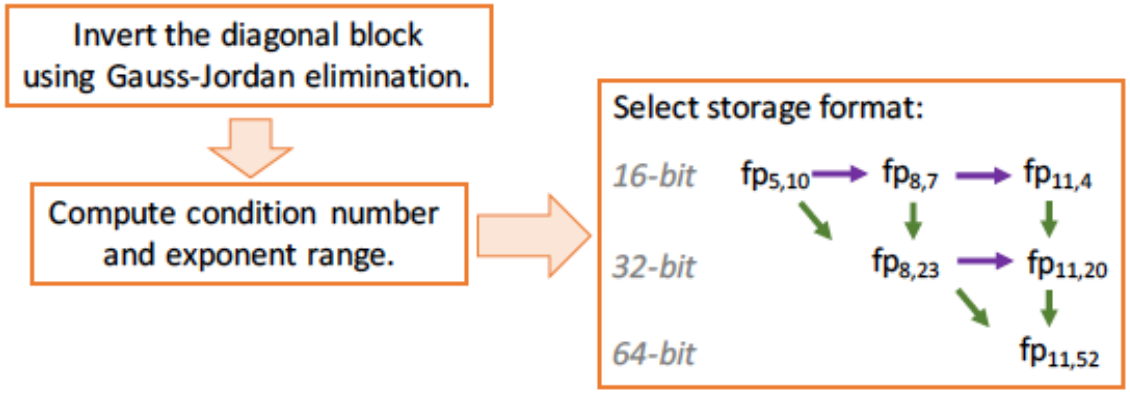
Idea: Store the inverted diagonal in low precision



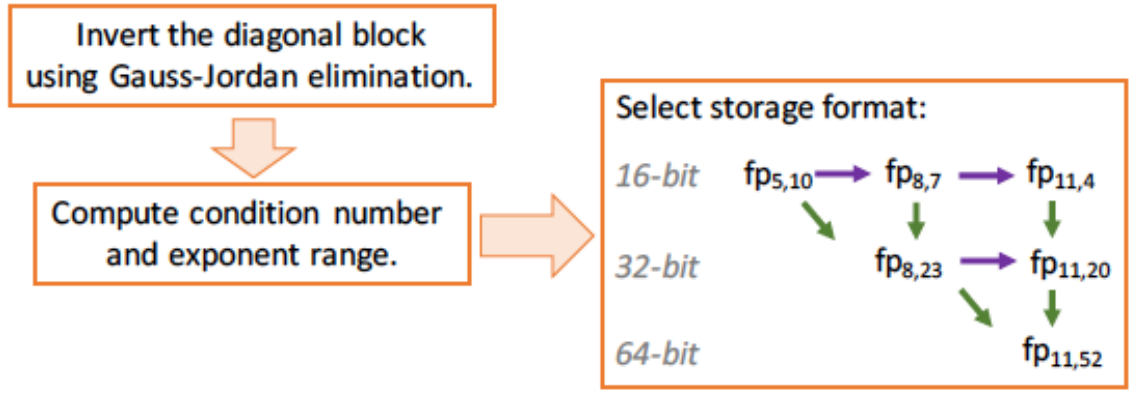
Adaptive Precision Preconditioning

- **Choose how much accuracy of the preconditioner should be preserved by the storage format.**
- **All computations use double precision, but store blocks in lower precision.**



Adaptive Precision Preconditioning

- **Choose how much accuracy of the preconditioner should be preserved by the storage format.** *2 digits*
- **All computations use double precision, but store blocks in lower precision.**



\+ **Regularity preserved;**

\+ Flexible in the accuracy preserved;

\+ No flexible Krylov solver needed

(Preconditioner constant operator);

\+ Can handle non-spd problems

(inversion features pivoting);

\+ Preconditioner for any iterative preconditionable solver;

\- **Overhead** of the **precision detection**

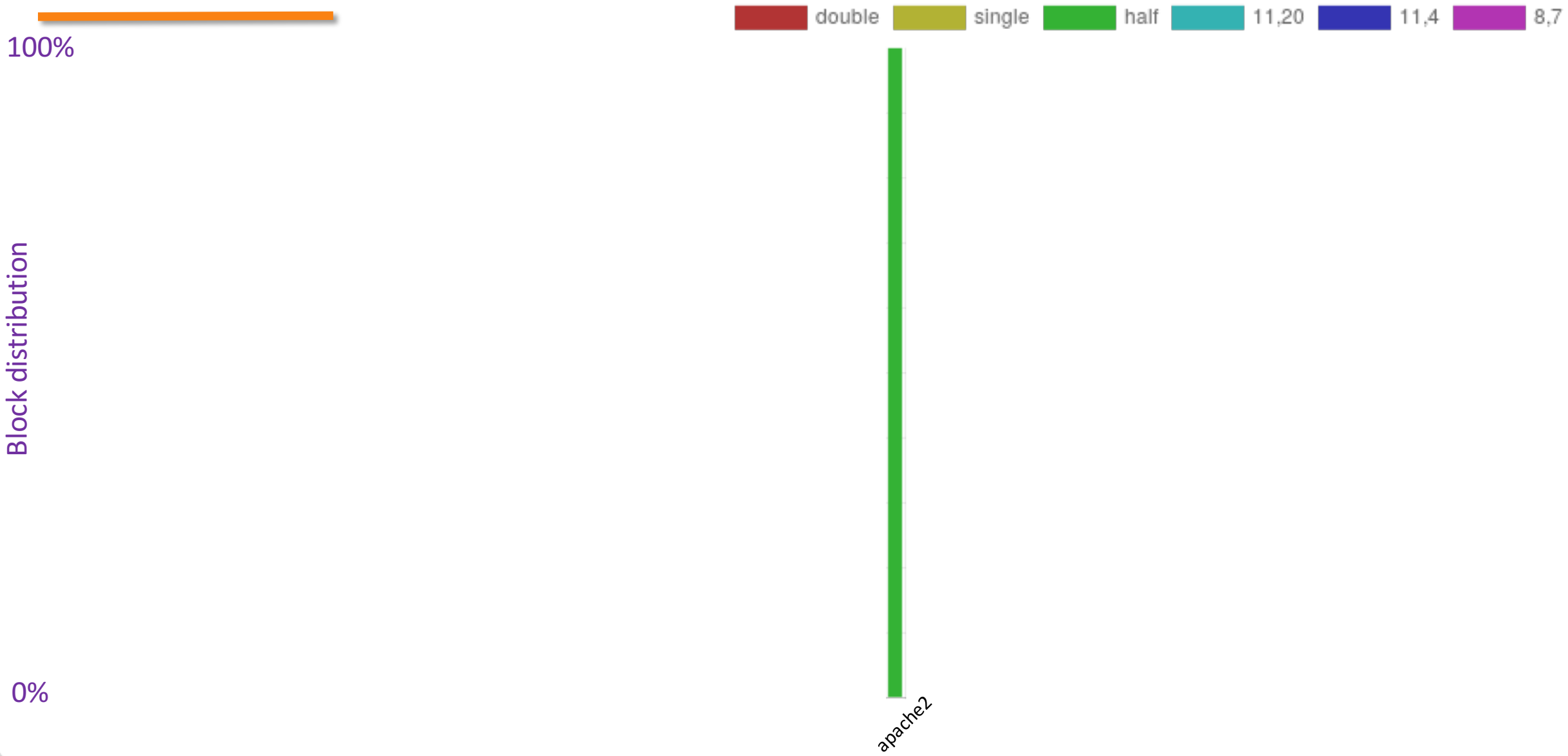
(condition number calculation);

\- **Overhead** from storing **precision information**

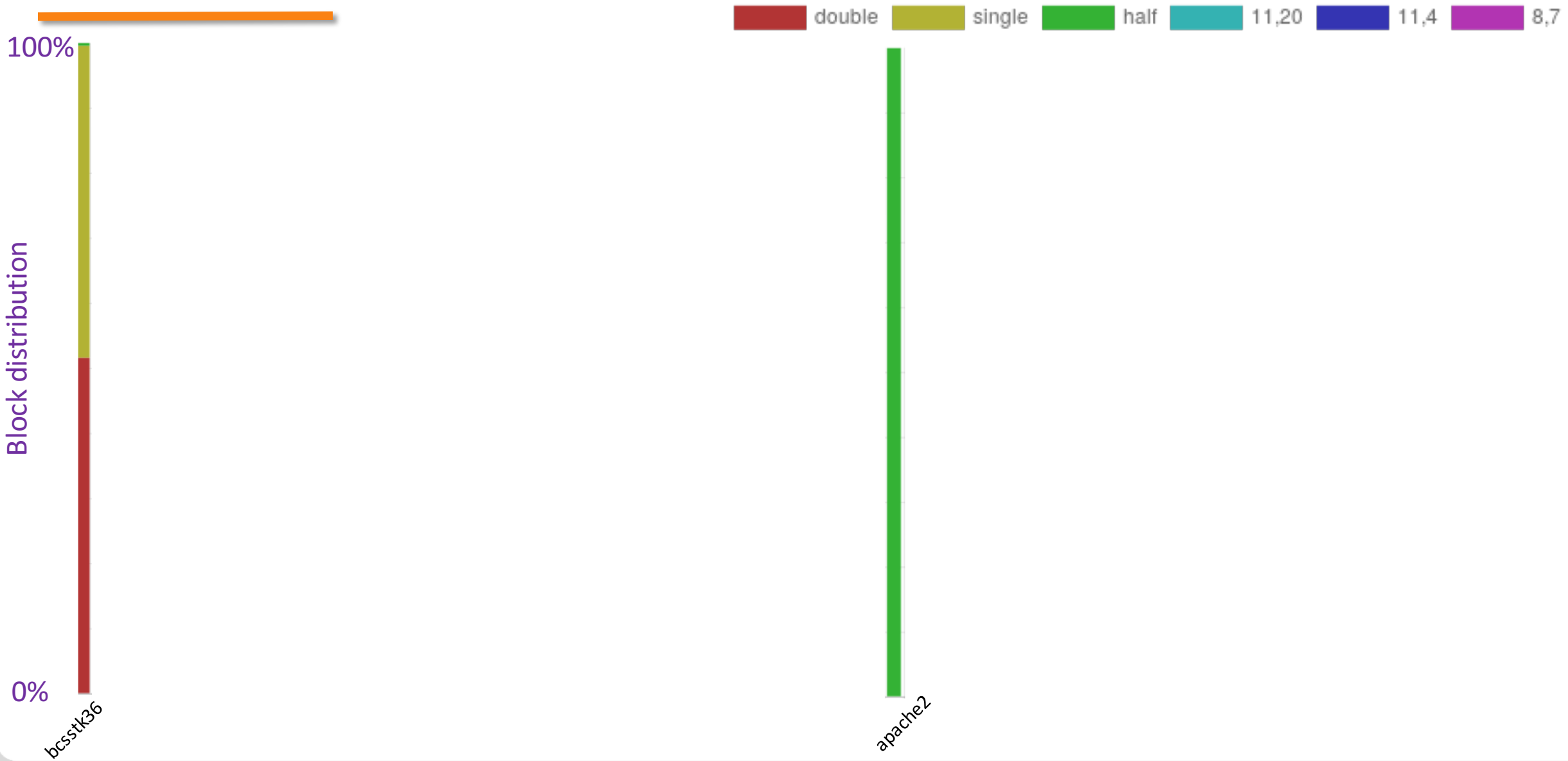
(need to additionally store/retrieve flag);

\- Speedups / preconditioner quality **problem-dependent**;

Adaptive Precision Preconditioning



Adaptive Precision Preconditioning



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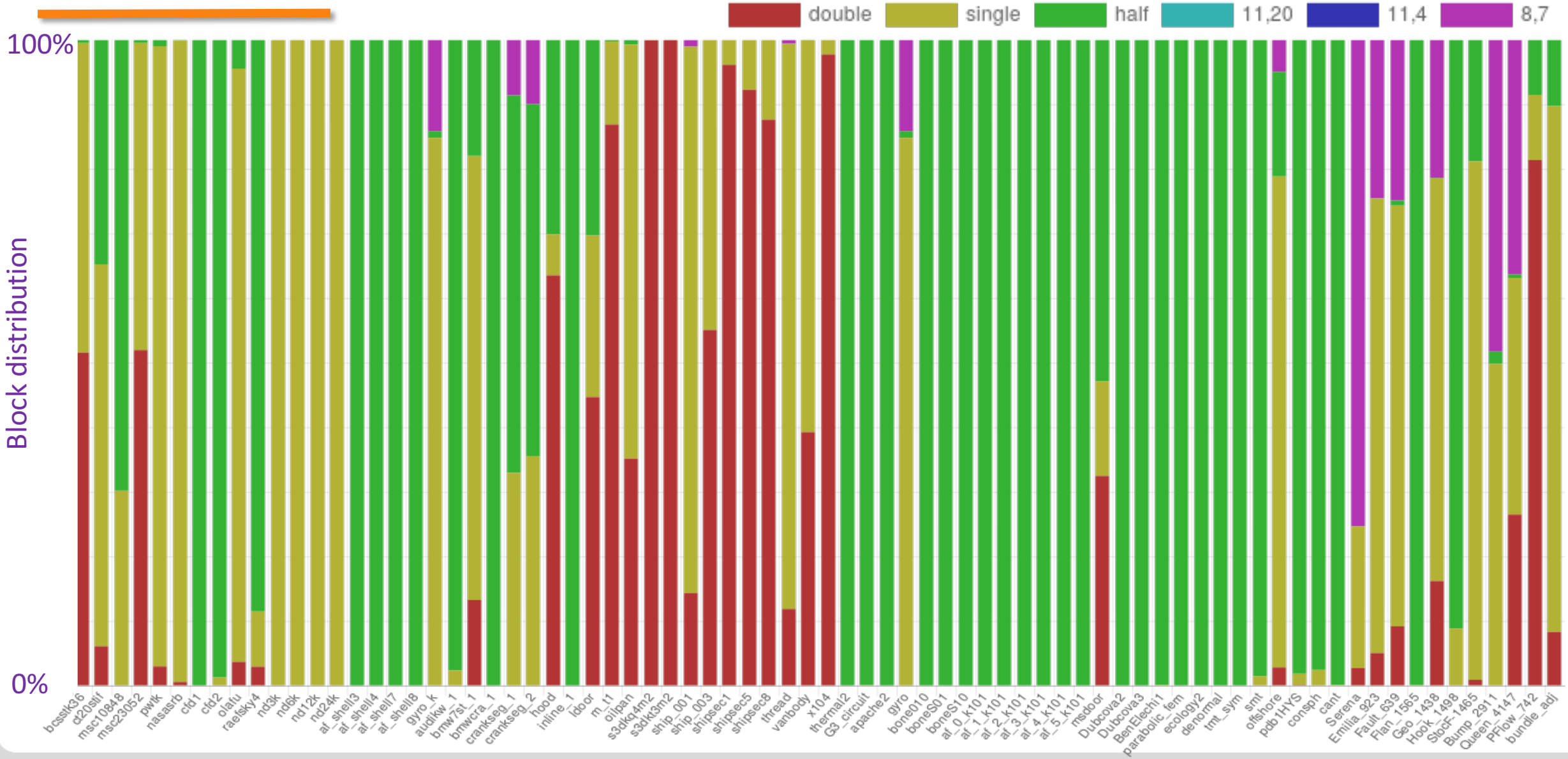


Floating point formats and accuracy

Linear System Ax=b with cond(A) ≈ 10^7

apache2 from SuiteSparse

Double Precision + Double Preconditioner

```
Initial residual norm sqrt(r^T r):
%%MatrixMarket matrix array real general
1 1
1390.67
Final residual norm sqrt(r^T r):
%%MatrixMarket matrix array real general
1 1
3.97985e-06
CG iteration count:     4797
CG execution time [ms]: 2971.18
```

Double Precision + Mixed Precision Preconditioner

```
Initial residual norm sqrt(r^T r):
%%MatrixMarket matrix array real general
1 1
1390.67
Final residual norm sqrt(r^T r):
%%MatrixMarket matrix array real general
1 1
3.98574e-06
CG iteration count:     4794
CG execution time [ms]: 2568.1
```

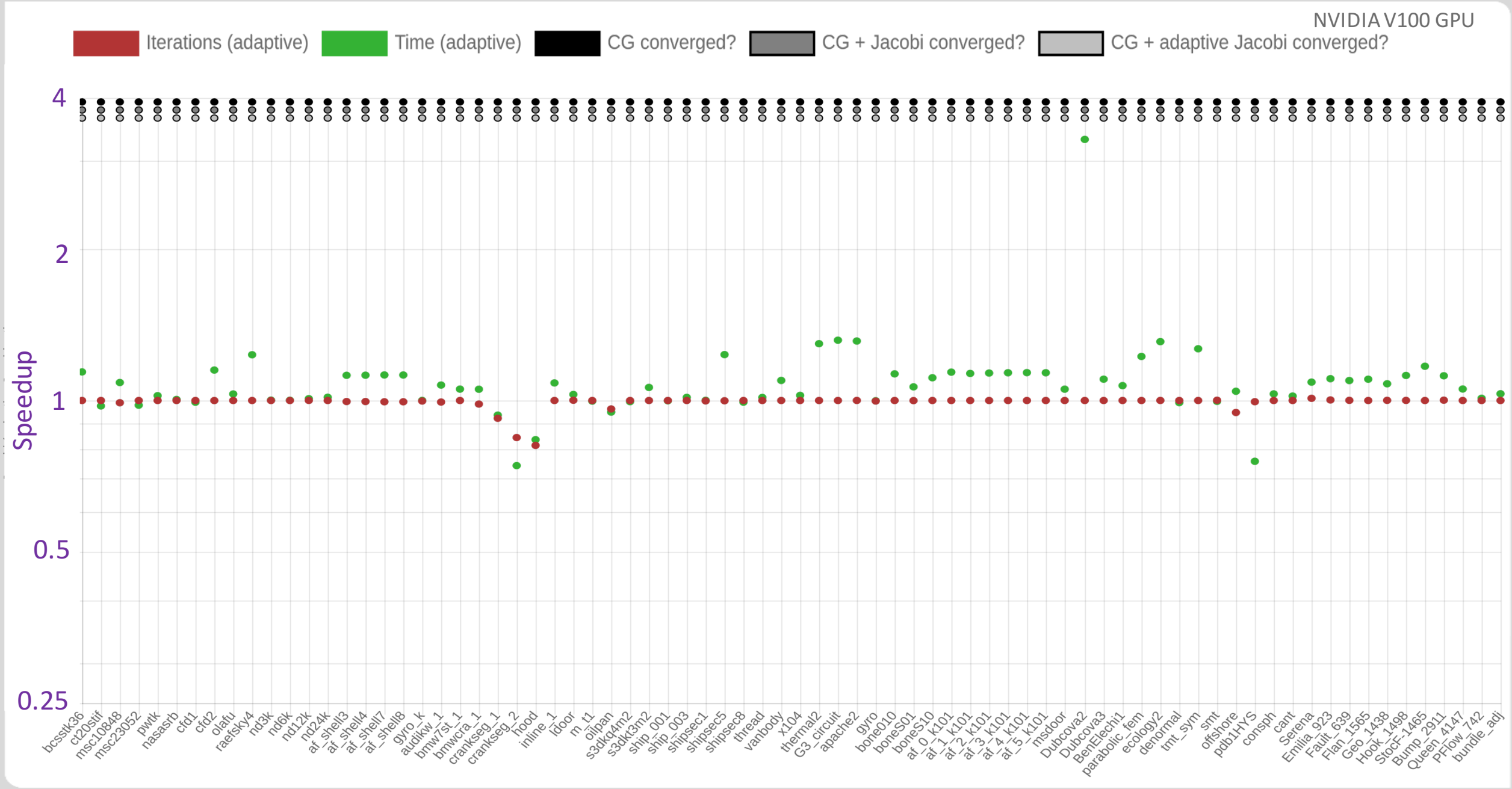
Experiments based on the Ginkgo library https://ginkgo-project.github.io/ginkgo/examples/adaptiveprecision-blockjacobi/adaptiveprecision-blockjacobi.cpp

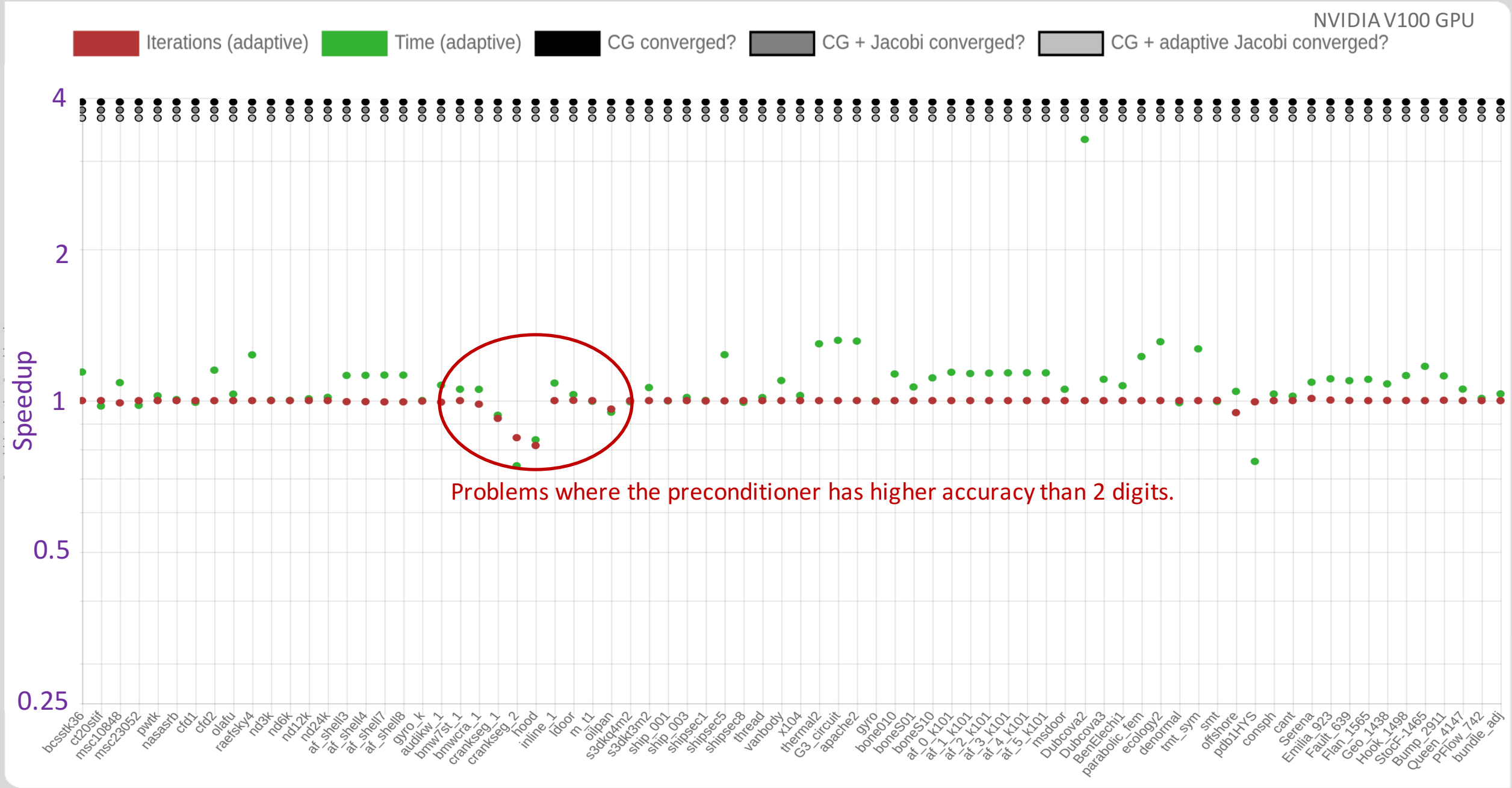
Floating point formats and accuracy

ginkgo/examples/adaptiveprecision-blockjacobi/adaptiveprecision-blockjacobi.cpp

```
…
    auto solver_gen =
            cg::build()
                .with_criteria(gko::share(iter_stop), gko::share(tol_stop))
                .with_preconditioner(bj::build()
                     .with_max_block_size(16u)
                     .with_storage_optimization(
                          gko::precision_reduction::autodetect())
                     .on(exec))
                .on(exec);
…
```

Experiments based on the Ginkgo library https://ginkgo-project.github.io/ginkgo/examples/adaptiveprecision-blockjacobi/adaptiveprecision-blockjacobi.cpp


NVIDIA V100 GPU
Iterations (adaptive)
Time (adaptive)
CG converged?
CG + Jacobi converged?
CG + adaptive Jacobi converged?
Speedup
4
2
1
0.5
0.25
Problem
bcsstk36
ct20stif
msc10848
msc23052
pwtk
nasasrb
cfd1
cfd2
olafu
raefsky4
nd3k
nd6k
nd12k
nd24k
af_shell3
af_shell4
af_shell7
af_shell8
gyro_k
audikw_1
bmw7st_1
bmwcra_1
crankseg_1
crankseg_2
hood
inline_1
ldoor
m_t1
oilpan
s3dkq4m2
s3dkt3m2
ship_001
ship_003
shipsec1
shipsec5
shipsec8
thread
vanbody
x104
thermal2
G3_circuit
apache2
gyro
boneS10
boneS01
boneS10
af_0_k101
af_1_k101
af_2_k101
af_3_k101
af_4_k101
af_5_k101
msdoor
Dubcova2
Dubcova3
BenElechi1
parabolic_fem
ecology2
denormal
tmt_sym
smt
offshore
pdb1HYS
consph
cant
Serena
Emilia_923
Fault_639
Flan_1565
Geo_1438
Hook_1498
StocF-1465
Bump_2911
Queen_4147
PFlow_742
bundle_adj


NVIDIA V100 GPU
Iterations (adaptive)
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CG converged?
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CG + adaptive Jacobi converged?
Speedup
4
2
1
0.5
0.25
Problems where the preconditioner has higher accuracy than 2 digits.
Problem
bcsstk36
ct20stif
msc10848
msc23052
pwtk
nasasrb
cfd1
cfd2
olafu
raefsky4
nd3k
nd6k
nd12k
nd24k
af_shell3
af_shell4
af_shell7
af_shell8
gyro_k
audikw_1
bmw7st_1
bmwcra_1
crankseg_1
crankseg_2
hood
inline_1
ldoor
m_t1
oilpan
s3dkq4m2
s3dkt3m2
ship_001
ship_003
shipsec1
shipsec5
shipsec8
thread
vanbody
x104
thermal2
G3_circuit
apache2
gyro
boneS10
boneS01
boneS10
af_0_k101
af_1_k101
af_2_k101
af_3_k101
af_4_k101
af_5_k101
msdoor
Dubcova2
Dubcova3
BenElechi1
parabolic_fem
ecology2
denormal
tmt_sym
smt
offshore
pdb1HYS
consph
cant
Serena
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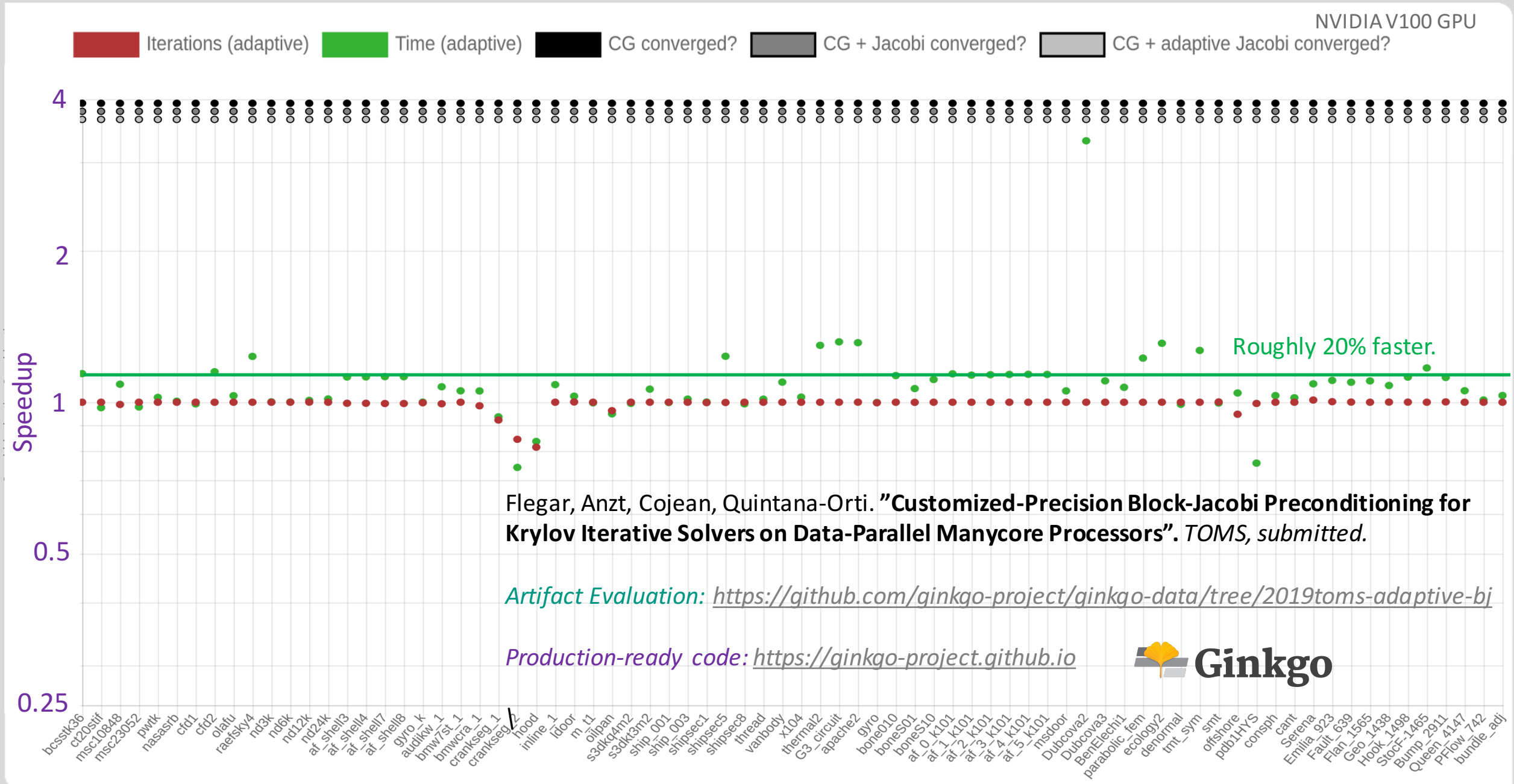
NVIDIA V100 GPU
Iterations (adaptive)
Time (adaptive)
CG converged?
CG + Jacobi converged?
CG + adaptive Jacobi converged?
Speedup
4
2
1
0.5
0.25
Roughly 20% faster.
Flegar, Anzt, Cojean, Quintana-Orti. "Customized-Precision Block-Jacobi Preconditioning for Krylov Iterative Solvers on Data-Parallel Manycore Processors". TOMS, submitted.
Artifact Evaluation: https://github.com/ginkgo-project/ginkgo-data/tree/2019toms-adaptive-bj
Production-ready code: https://ginkgo-project.github.io
Ginkgo
Problem

Take-Away

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- Performance of **memory-bound** algorithms scales hardware-independent with **inverse of format complexity**.
- **relative residual accuracy** = **(unit round-off)** * **(linear system's condition number)**
- If the problem is **well-conditioned**, and a **low-accuracy solution is acceptable**, use a **low precision format**. (i.e. IEEE single precision, or even IEEE half precision.)
- **Low precision preconditioners** can be used to **accelerate iterative solvers**.
  - Adapt precision to numerical requirements and preconditioner quality.
- **To increase the performance benefits, shift most of the work to the low precision preconditioner.**

Using a low precision solver as preconditioner

- **To increase the performance benefits, shift most of the work to the low precision preconditioner.**

- Use a **simple (cheap) iterative solver** in **high precision**
  and a **sophisticated (expensive) solver** in **low precision** as preconditioner.
  - Most of the work is done in low precision (fast).
  - The high precision outer solver ensures high quality of the solution.

- Popular example: Iterative Refinement *(see Jack Dongarra's talk)*

  For an approximate solution $x^{(k)}$, the residual computes as $r = b - Ax^{(k)}$.
  The exact solution for $Ax = b$ is $x = x^{(k)} + c$ where c is the solution of $Ac = r$.

Iterative Refinement

```
Choose initial guess x
do {
        Compute r = b - Ax
        Solve A * c = r
        Update x = x + c
} while ( ||r||>tol )
```

Using a low precision solver as preconditioner

- **To increase the performance benefits, shift most of the work to the low precision preconditioner.**

- Use a **simple (cheap) iterative solver** in **high precision**
  and a **sophisticated (expensive) solver** in **low precision** as preconditioner.
  - Most of the work is done in low precision (fast).
  - The high precision outer solver ensures high quality of the solution.

- Popular example: Iterative Refinement *(see Jack Dongarra's talk)*

For an approximate solution $x^{(k)}$, the residual computes as $r = b - Ax^{(k)}$.
The exact solution for $Ax = b$ is $x = x^{(k)} + c$ where c is the solution of $Ac = r$.

Mixed Precision Iterative Refinement

```
Choose initial guess x          high precision
do {
        Compute r = b - Ax      high precision
        Solve A * c = r         low precision
        Update x = x + c        high precision
} while ( ||r||>tol )           high precision
```

N. Higham: Accuracy and stability of numerical algorithms. SIAM, 2002.

Sri Pranesh's mixed precision Matlab suite:
https://github.com/SrikaraPranesh/Multi_precision_NLA_kernels

Mixed Precision Iterative Refinement using sparse iterative solvers

Linear System Ax=b with cond(A) ≈ 10^4

Double Precision

```
Initial residual norm sqrt(r^T r):
%%MatrixMarket matrix array real general
1 1
111.127
Final residual norm sqrt(r^T r):
%%MatrixMarket matrix array real general
1 1
5.0775e-10
CG iteration count:     1231
CG execution time [ms]: 140.038
```

Accuracy improvement ~10^{13}

Single Precision

```
Initial residual norm sqrt(r^T r):
%%MatrixMarket matrix array real general
1 1
111.127
Final residual norm sqrt(r^T r):
%%MatrixMarket matrix array real general
1 1
0.179829
CG iteration count:     1234
CG execution time [ms]: 127.152
```

Accuracy improvement ~10^4

relative residual accuracy = (unit roundoff) * (linear system's condition number)

Experiments based on the Ginkgo library https://ginkgo-project.github.io/ginkgo/examples/mixed-precision-ir/mixed-precision-ir.cpp

Mixed Precision Iterative Refinement using sparse iterative solvers

Linear System Ax=b with cond(A) ≈ 10^4

Double Precision Iterative Refinement

```
Initial residual norm sqrt(r^T r):
%%MatrixMarket matrix array real general
1 1
111.127
Final residual norm sqrt(r^T r):
%%MatrixMarket matrix array real general
1 1
7.16102e-11
MPIR iteration count:     18
MPIR execution time [ms]: 213.491
```

Accuracy improvement ~10^{14}

Mixed Precision Iterative Refinement

```
Initial residual norm sqrt(r^T r):
%%MatrixMarket matrix array real general
1 1
111.127
Final residual norm sqrt(r^T r):
%%MatrixMarket matrix array real general
1 1
7.41333e-11
MPIR iteration count:     18
MPIR execution time [ms]: 183.296
```

Accuracy improvement ~10^{14}

16% runtime improvement

Experiments based on the Ginkgo library https://ginkgo-project.github.io/ginkgo/examples/mixed-precision-ir/mixed-precision-ir.cpp

Mixed Precision Iterative Refinement using sparse iterative solvers

L

Some references:

Strzodka et al. **Pipelined Mixed Precision Algorithms on FPGAs for Fast and Accurate PDE Solvers from Low Precision Components**, IEEE Symposium on Field-Programmable Custom Computing Machines, 2006.

Goedekke et al. **Performance and accuracy of hardware-oriented native-, emulated- and mixed-precision solvers in FEM simulations**, International Journal of Parallel, Emergent and Distributed Systems, 2007.

Buratti et al. **Using Mixed Precision for Sparse Matrix Computations to Enhance the Performance while Achieving 64-bit Accuracy**, ACM TOMS 2008.

Baboulin et al. **Accelerating scientific computations with mixed precision algorithms**, CPC, 2009.

Anzt et al. **Mixed precision iterative refinement methods for linear systems: Convergence analysis based on Krylov subspace methods**, PARA 2010.

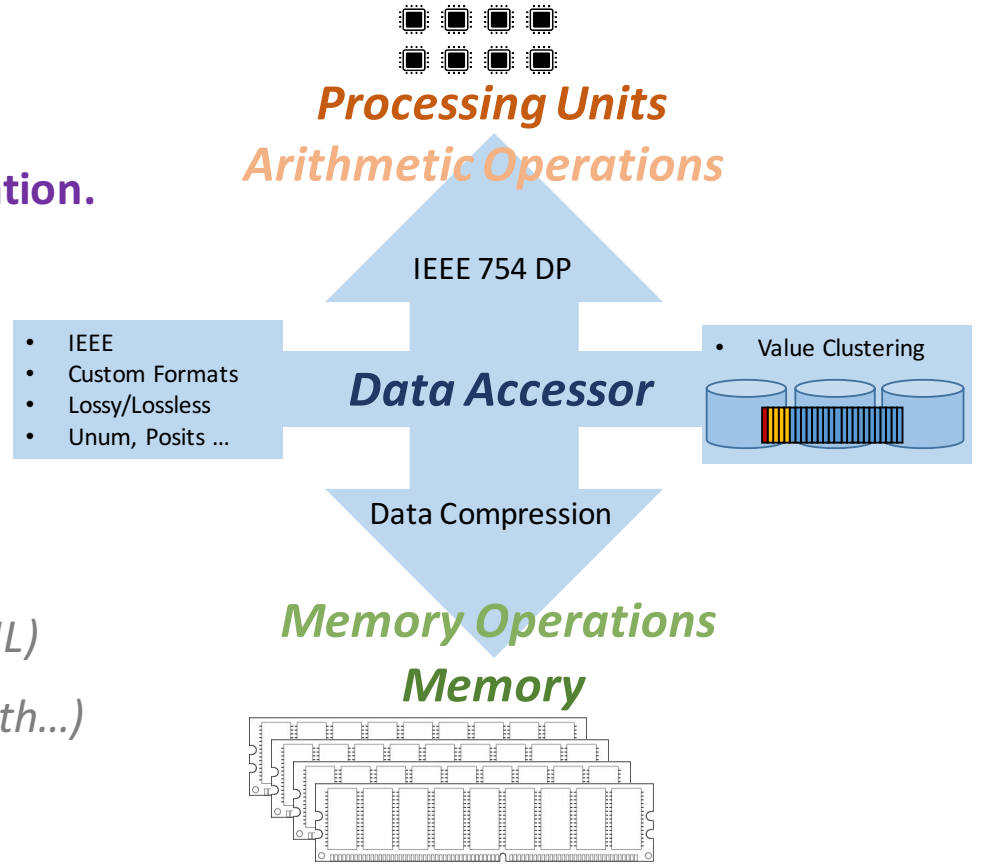
…

- **For sparse iterative methods, the benefits relate to the bandwidth savings;**

E

Future plans for sparse methods using mixed precision

- **Decouple arithmetic precision from memory precision / communication.**
- Using **customized precisions** for memory operations.
- Use problem-adapted **lower precision in preconditioning**
  - *Adaptive precision block-Jacobi / SAI*
  - *ILU preconditioning*
  - *Mixed Precision Iterative Refinement*
  - *Multigrid (Ulrike Meier Yang@LLNL …)*
  - *Polynomial preconditioning (Jennifer Loe and Erik Boman @ SNL)*
- **Mixed precision Krylov solvers** *(Erin Carson, Steve Thomas, Barry Smith…)*
- **Mixed Precision Sparse LU** *(Sherry Li…)*



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