Restoring Reproducibility to Lattice QCD

Kate Clark, Lattice 2023

Motivation

- Floating point arithmetic is non-associative

$$(a + b) + c \neq a + (b + c)$$

- Parallel reductions will yield different answers whenever we change otherwise seemingly innocuous parameters
- Is this a problem?
  - Won’t answers only be different to floating point epsilon?
- Lattice QCD calculations can exhibit chaotic behavior
  - Small changes can cause divergent HMC phase space traversal
- Without exact reproducibility we lose the ability to repeat experiments (simulations)
  - This is a failure of the scientific method
  - To fully specify a given physics ensemble, one would need to fully specify the order of all summation operations
  - Debugging….

Sources of Chaos

- Data ordering
  - Structure of Arrays vs Array of Structures vs SIMD ordering
- Architecture specifics
  - Floating point rounding employed
  - Flush denormals to zero?
- Multi-process decomposition
  - Number of processes
  - Process grid (e.g., 4x4x4x4 vs 2x4x4x8)
- Hierarchical many-core processors (GPUs)
  - Thread block size
  - Number of thread blocks
  - Work items per thread
- Stencil application (Dslash)
  - Local gather vs halo gather

**ECP benchmarks apps

EXASCALE COMPUTING PROJECT

SciDAC
Scientific Discovery through Advanced Computing

QUDA

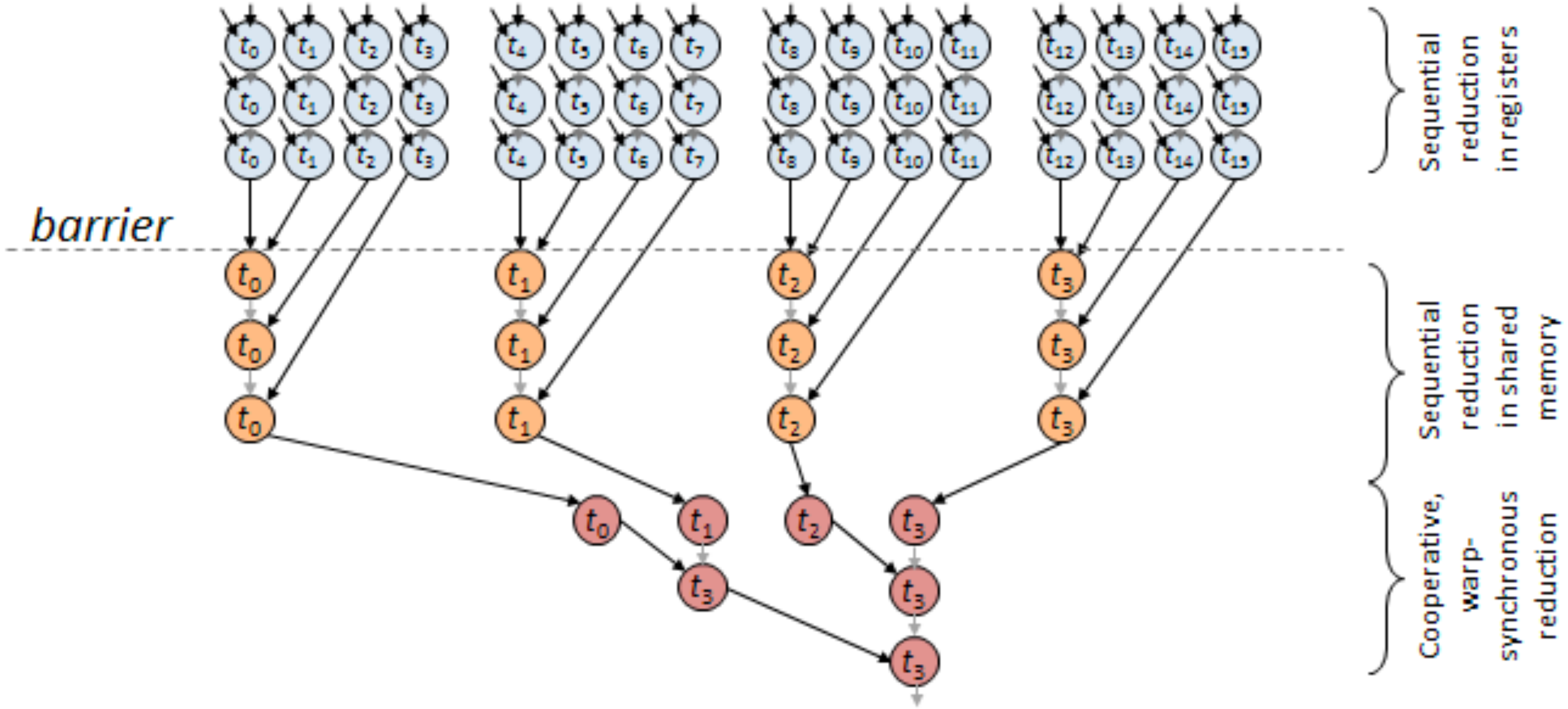
- “QCD on CUDA” – http://lattice.github.com/quda (open source, BSD license)
- Effort started at Boston University in 2008, now in wide use as the GPU backend for BQCD, **Chroma**, CPS**, MILC****, TIFR, etc.
- Provides solvers for major fermionic discretizations, pure gauge algorithms, etc.
- Maximize performance
  - Mixed-precision methods
  - Autotuning for high performance on all CUDA-capable architectures
  - Multigrid solvers for optimal convergence
  - NVSHMEM for improving strong scaling
- Portable: HIP (merged), SYCL (in review) and OpenMP (in development)
- **A research tool for how to reach the exascale (and beyond)**
  - Optimally mapping the problem to hierarchical processors and node topologies

Tree Reduction Algorithm

- Classic parallel reduction algorithm
  - For data set v[N], launch N/2 threads
  - Each thread performs pairwise reduction u[t] = reduce(v[t], v[t + N/2])
  - Store result and repeat with half the number of threads
  - Complete reduction performed in log(N) steps

- Modern optimized form
  - Fixed set of T threads rake over the data
  - Each thread accumulates N/T terms locally
  - Then perform tree summation between threads

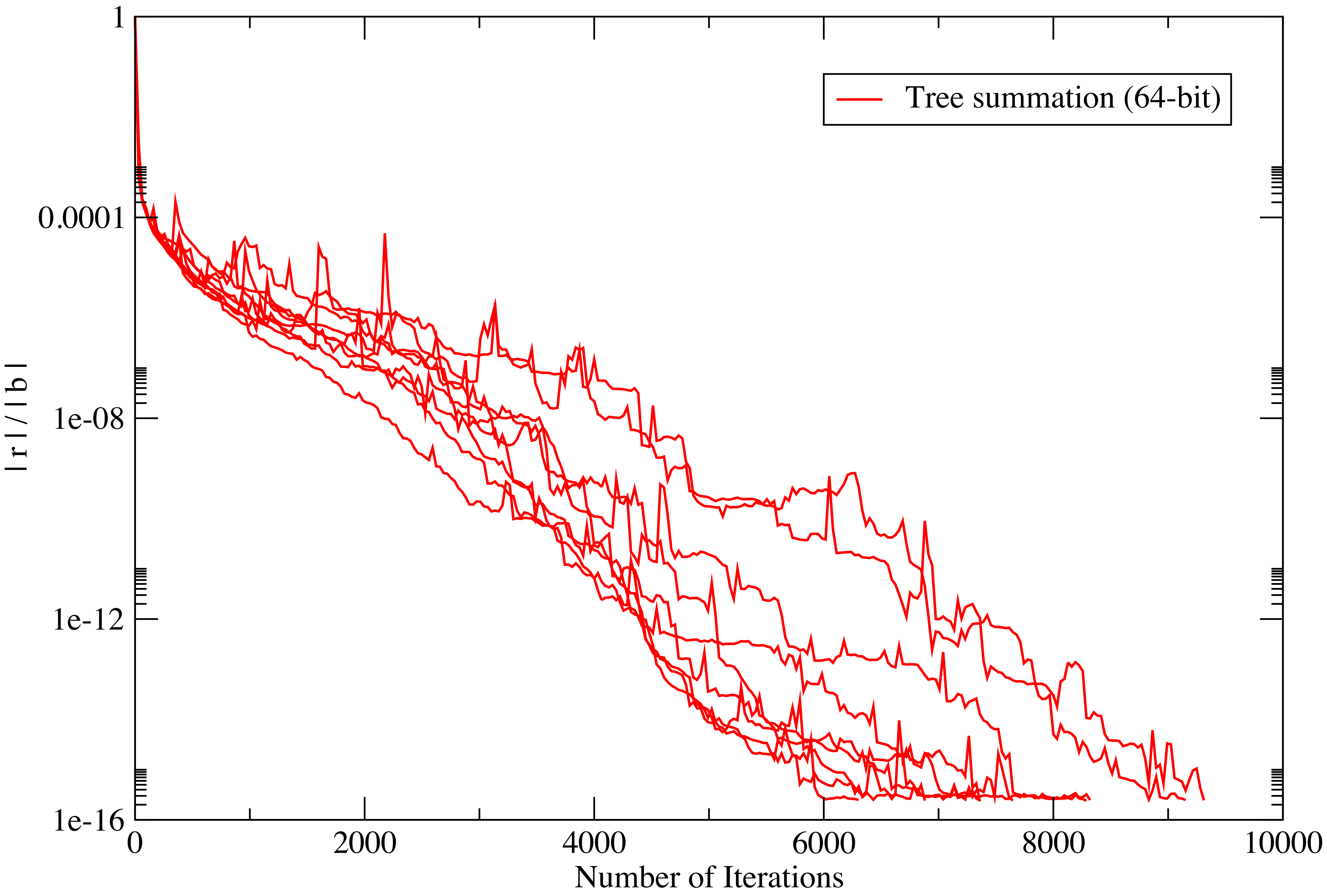
- If we change T we will alter the order of summation…



https://github.com/NVIDIA/cub

Solver Chaos

- Run same solver 10 times with different GPU thread counts
- BiCGStab(l) with Wilson fermions
  - $V = 16^3 x64$
  - 2 MPI processes, 2 GPUs
  - Target relative residual $2x10^{-16}$
- Double precision reductions
  - 9 unique convergence histories
- Residual is insensitive to low-mode errors
  - “Equivalent” solutions may have drastically different error components
  - Low modes “tickle” instabilities in the MD integration



Can we fix it using higher precision?

- Double precision is not the limit

```
struct float64_t {
  unsigned int mantissa : 52;
  unsigned int exponent : 11;
  unsigned int sign     :  1;
};
```

```
struct float128_t {
  unsigned int mantissa : 113;
  unsigned int exponent :  15;
  unsigned int sign     :   1;
};
```

IEEE binary64

64-bits per real

53-bit mantissa => Precision $\varepsilon \sim 1 \times 10^{-16}$

8-bit exponent => Range $\in [2 \times 10^{-208}, 2 \times 10^{308}]$

IEEE binary128

128-bits per real

113-bit mantissa => Precision $\varepsilon \sim 2 \times 10^{-34}$

15-bit exponent => Range $\in [3 \times 10^{-4932}, 1 \times 10^{4932}]$

- Most modern processors do not support IEEE fp128........

Double-double

- Use two doubles to emulate a quad
  - Effective 107 bits of precision (nearly as much as binary128)

- double-double addition operation costs 20 double precision additions
  - But flops are free and everything's bandwidth?

Double-double addition function

```
/* Compute high-accuracy sum of two double-double operands. In the absence of
   underflow and overflow, the maximum relative error observed with 10 billion
   test cases was 3.0716194922303448e-32 (~= 2**-104.6826).
   This implementation is based on: Andrew Thall, Extended-Precision
   Floating-Point Numbers for GPU Computation. Retrieved on 7/12/2011
   from http://andrewthall.org/papers/df64_qf128.pdf.
*/
__device__ __host__ __forceinline__ dbldbl add_dbldbl (dbldbl a, dbldbl b)
{
    dbldbl z;
    double t1, t2, t3, t4, t5, e;
    t1 = dadd_rn (a.y, b.y);
    t2 = dadd_rn (t1, -a.y);
    t3 = dadd_rn (dadd_rn (a.y, t2 - t1), dadd_rn (b.y, -t2));
    t4 = dadd_rn (a.x, b.x);
    t2 = dadd_rn (t4, -a.x);
    t5 = dadd_rn (dadd_rn (a.x, t2 - t4), dadd_rn (b.x, -t2));
    t3 = dadd_rn (t3, t4);
    t4 = dadd_rn (t1, t3);
    t3 = dadd_rn (t1 - t4, t3);
    t3 = dadd_rn (t3, t5);
    z.y = e = dadd_rn (t4, t3);
    z.x = dadd_rn (t4 - e, t3);
    return z;
}
```

Reworking QUDA's Reductions…

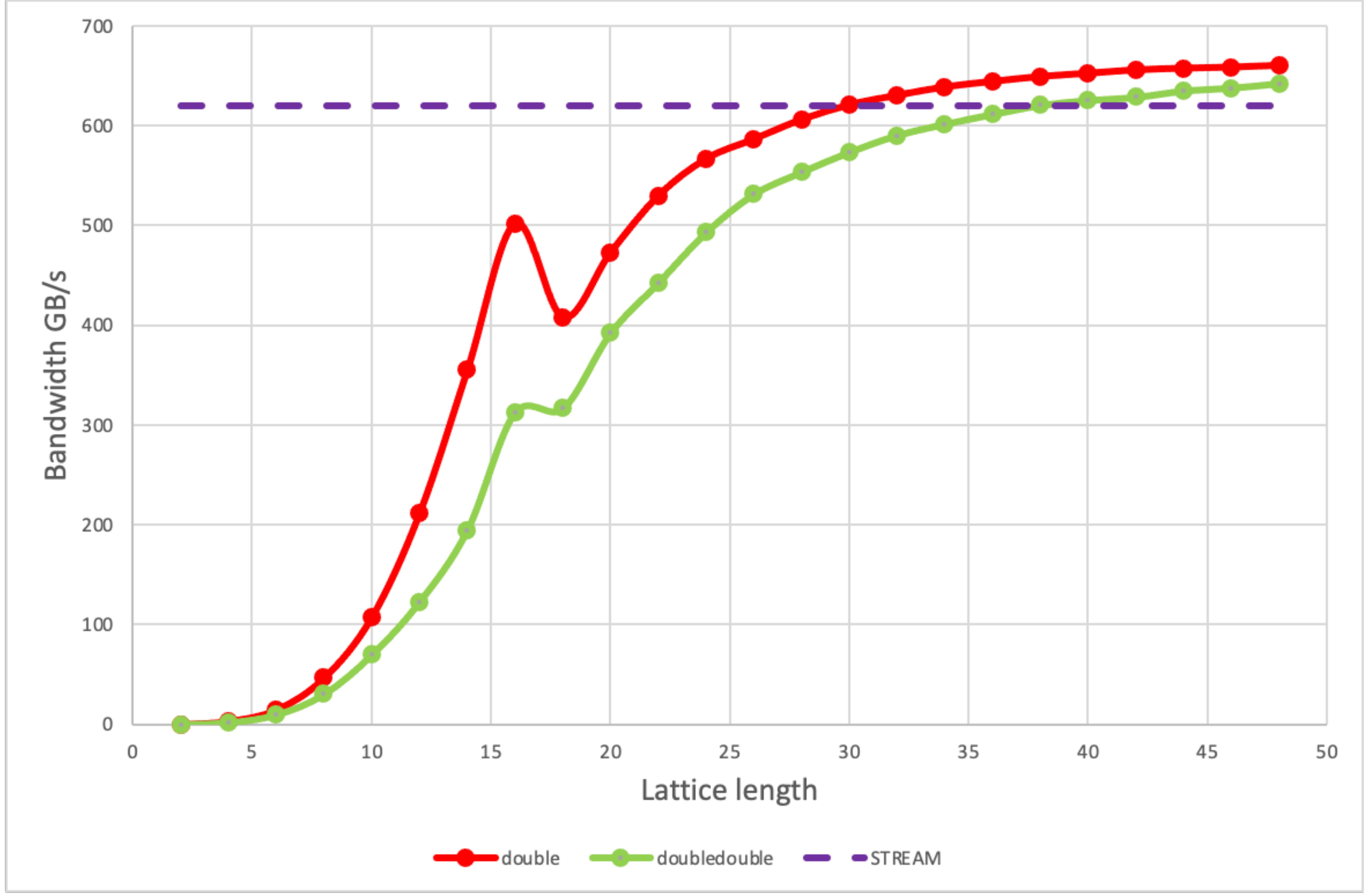
- Old
    - Host types hard coded to double precision
    - Only naive tree summation algorithm implemented

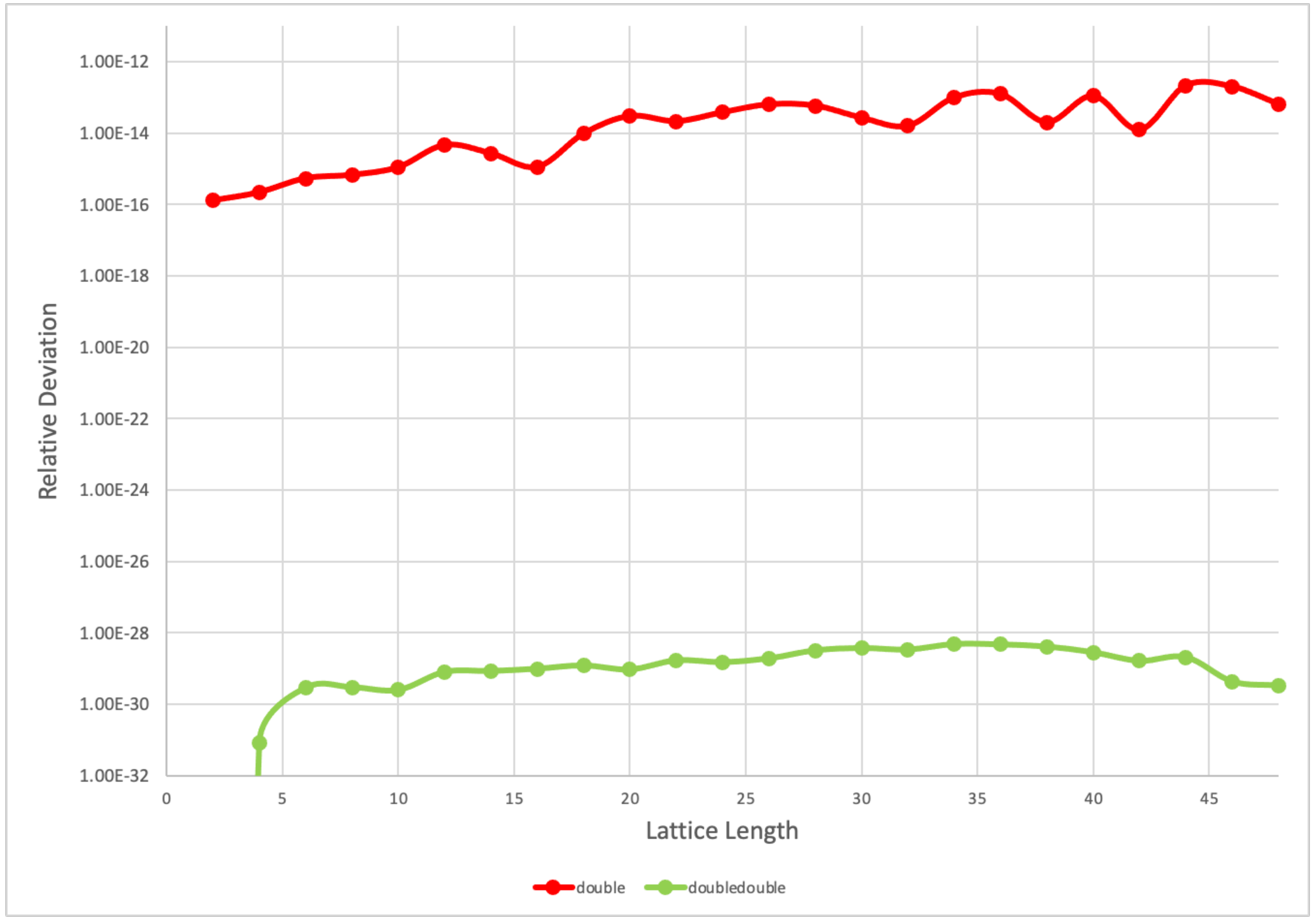
- New abstraction
    - Reduction type
        - Defines the precision of any sum reductions
    - Separate type for host scalar type
        - e.g., CG's alpha, beta coefficients
    - Parallel summation algorithm
        - e.g., naive, Kahan, reproducible
    - All configured by CMake build system

Double-double Reductions

QUDA Implementation

Asymptotic 3% overhead





Performance on Norm2 reduction kernel, fp64 inputs (Quadro GV100, CUDA 12.1)

Relative Deviation between CPU and GPU Norm2 reductions

Solver Chaos

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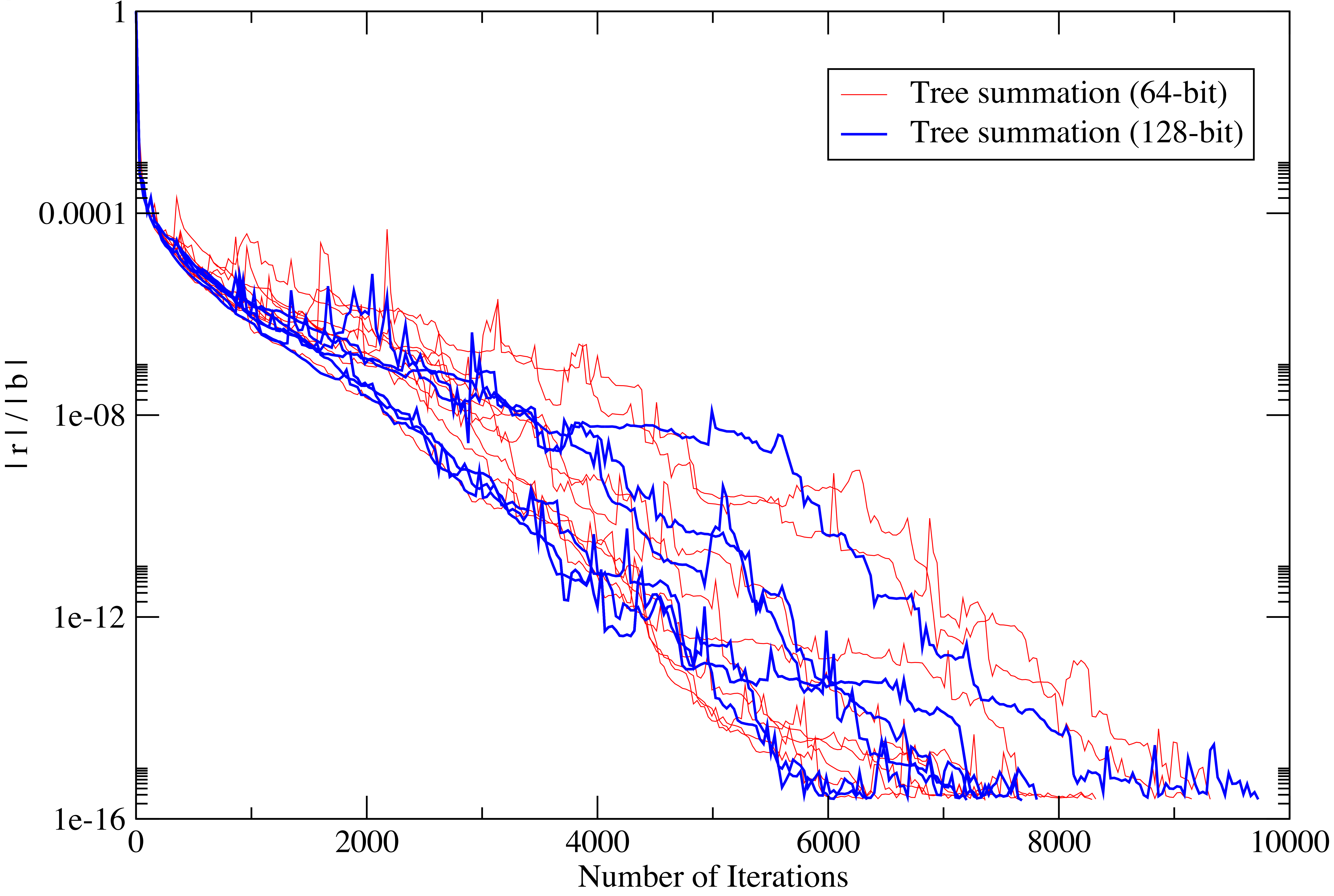
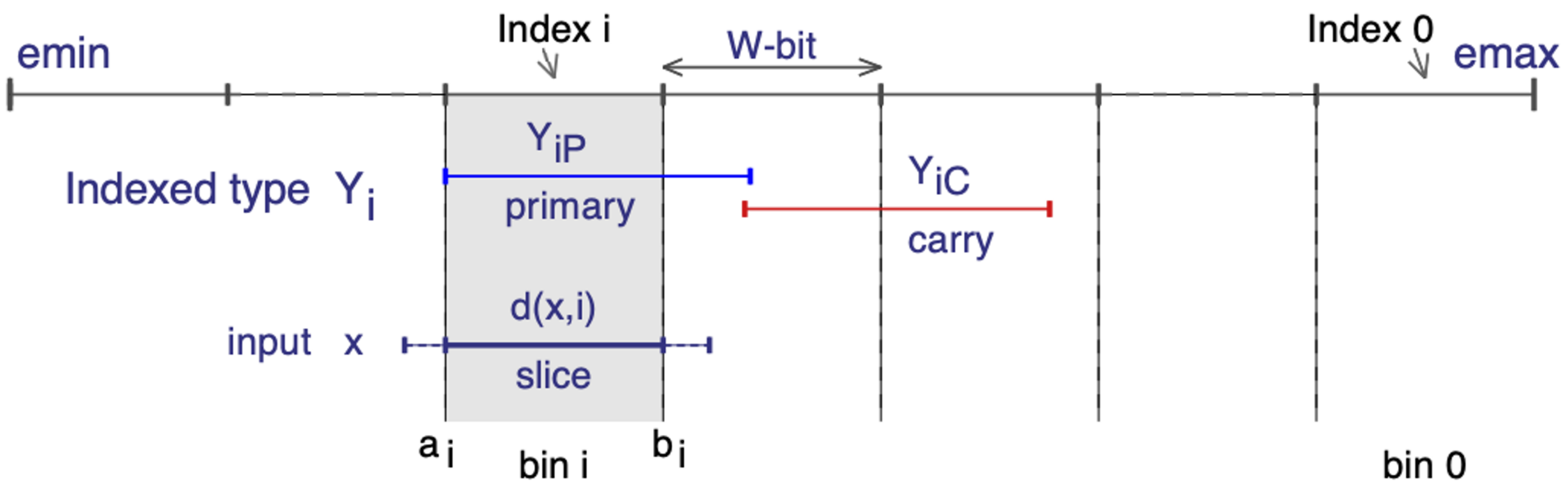
- Double-double reductions
  - 6 unique convergence histories



https://doi.org/10.1145/3389360

Reproducible Summation

Ahrens *et al*, 2020



- Reproducible Summation (aka K-fold summation)
  - Bin the components of each number into bins of predefined exponent range
  - Each binned component is known as a “slice”
- We can sum the slices in the same bin *exactly*, so long as we don’t overflow
  - Abusing floating point to behave as integer (integer is associative)
  - Given a bin width of **W** bits, and precision **P** bits, we can sum $\mathbf{2^{P-W}}$ slices exactly
    - E.g., FP32 (single precision)
      - P = 24, W = 13
      - We can add 2^{11} slices together *exactly*

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Reproducible Summation

Ahrens *et al*, 2020

- When summing slices, each summation represented by two bins:
  - Primary: where each slice's value is summed to
  - Carry: store any overflow bits from summation to primary

- Algorithm is exact if we fully cover the range of the underlying floating-point representation
  - Not feasible for double precision (way too many bins required)

- Only retain a fixed number of bins K (typically $K = 3$)
  - So each real number requires K x (primary + carry) values

- Maximum bin based on set maximum value
  - Avoid pre-computing the set maximum by tracking maximum value to date
  - If new maximum encountered shift bins and drop least significant bins as needed

- Once summation of slices is complete, reconstruct the final floating point value

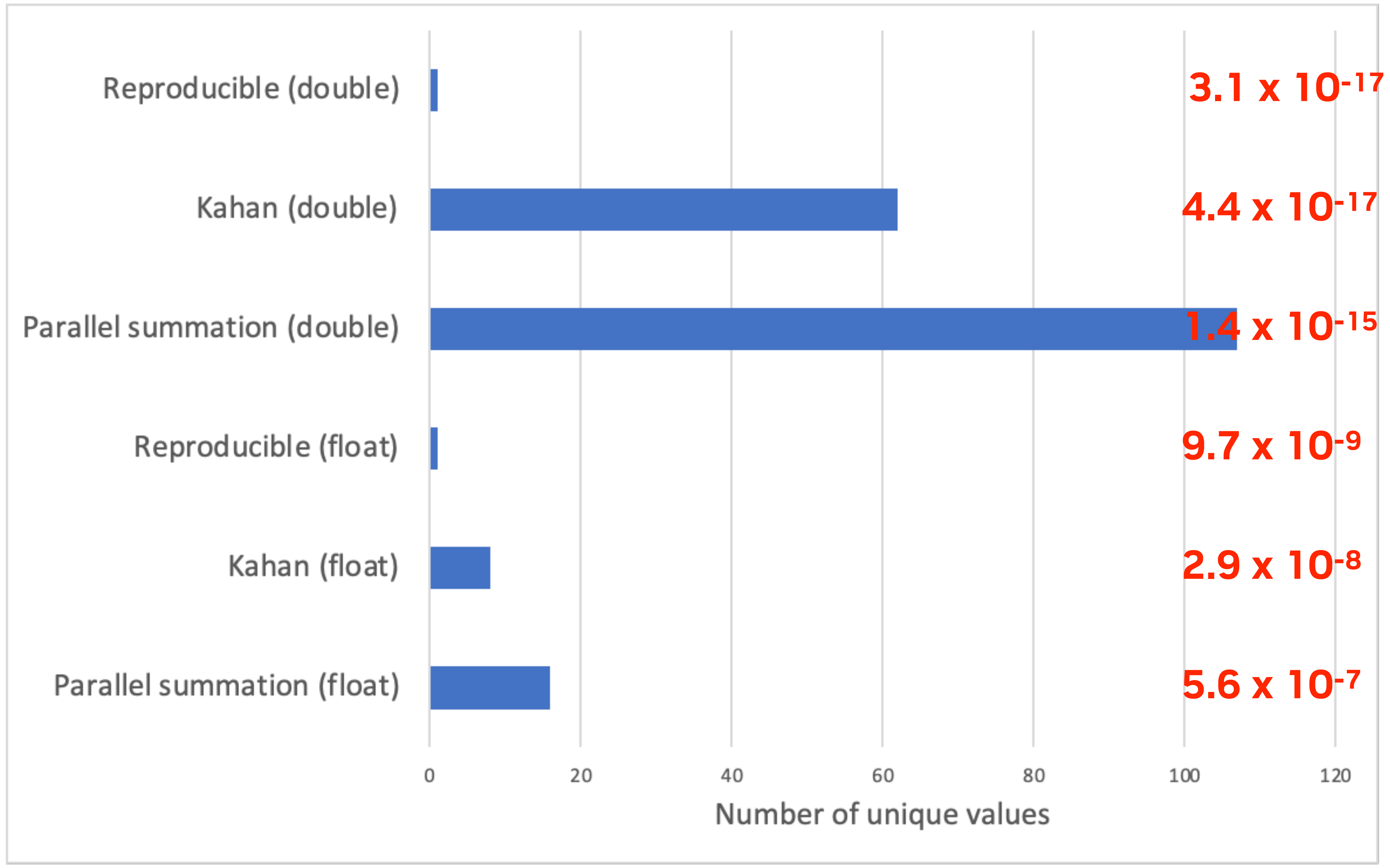
- Absolute error bound: $E \leq 2^{-(K-1)W} N \mathbf{max}\, x_i$
  - FP64: $E \leq 2^{-27} \varepsilon N \mathbf{max}\, x_i \quad (K = 3, W = 40)$
  - Compared to standard summation $E \leq (N-1)\,\varepsilon \sum_i \|x_i\|$

Reproducible Summation

- Compare summation of same set under a random permutation
- Compare to exactly computed reference

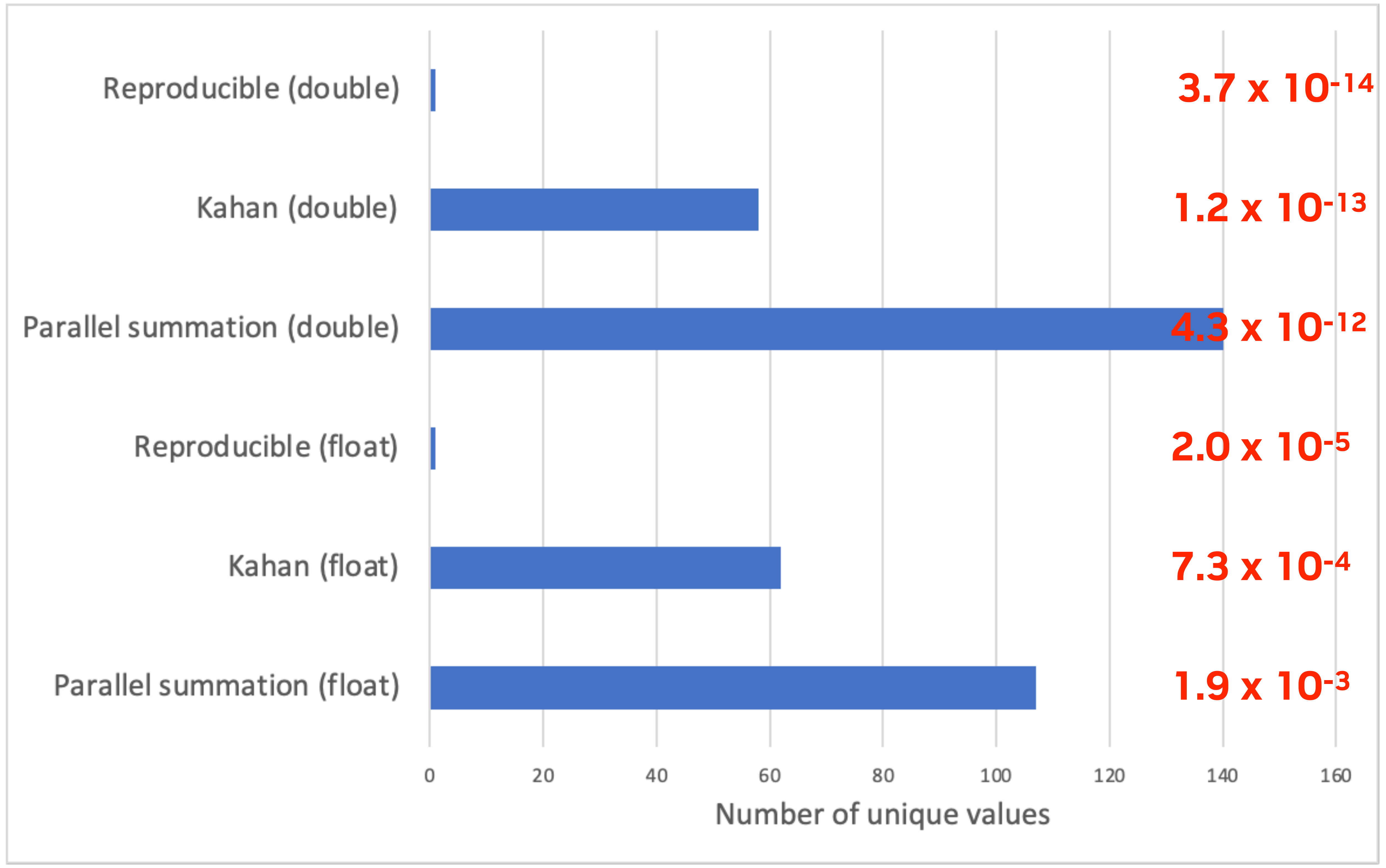
Positive Uniform Random (N = 10^7, 1000 permutations)

Maximum Relative Error



Sine Wave (N = 10^7, 1000 permutations)

Maximum Absolute Error



Reproducible Summation on GPUs

Algorithm as presented not efficient for parallel architectures

```
return p[index];
```

```
switch (index) {
case 0: return p[0];
case 1: return p[1];
case 2: return p[2];
case 3: return p[3];
case 4: return p[4];
}
```

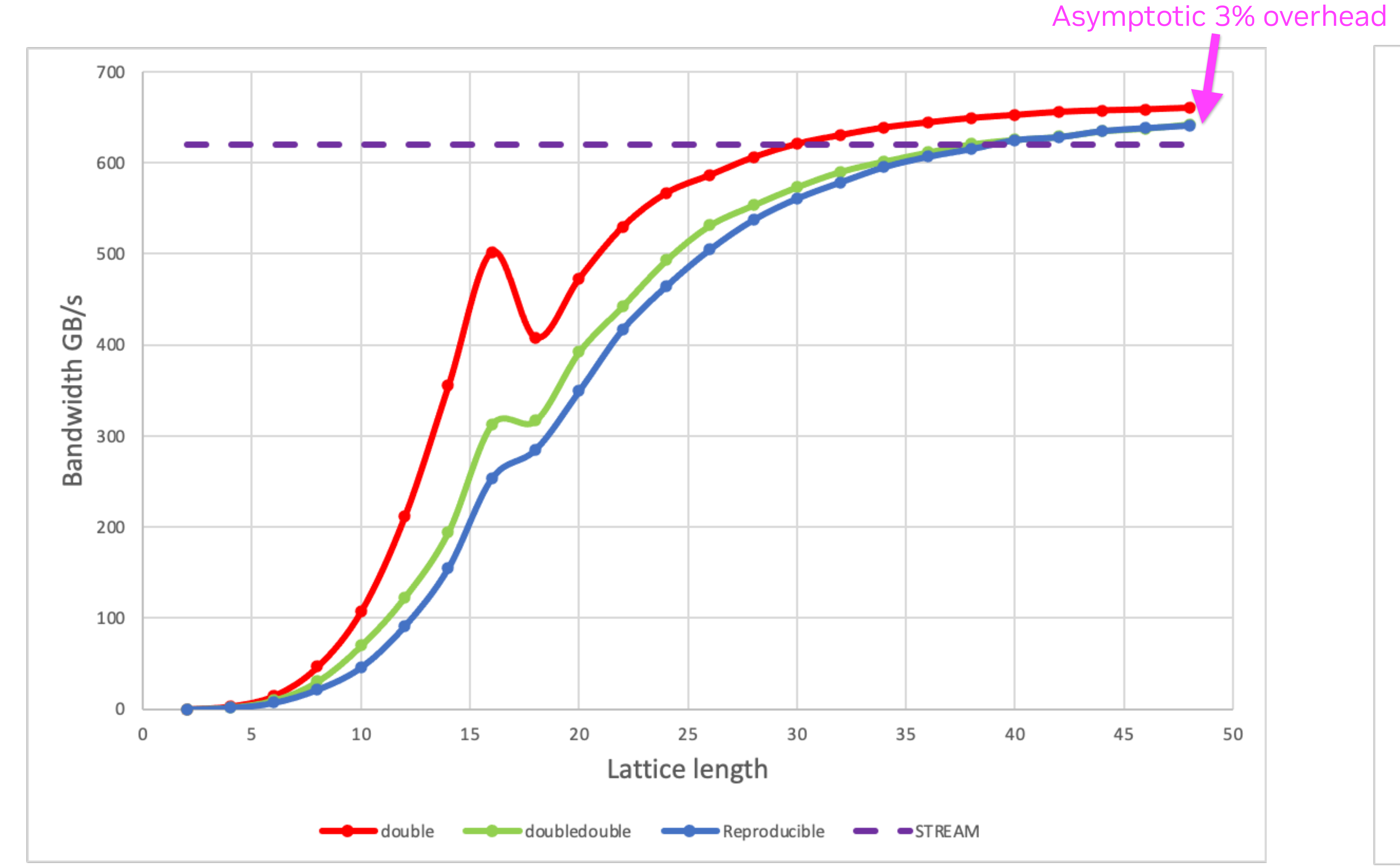
- Thread bin indices computed dynamically based on present summand value
  - Cannot dynamically index registers leading to spilling of bins into cache hampering performance
  - Solution: use switch table instead of direct array indexing

- Each thread’s local maximum may differ dramatically
  - Bin shifting overhead when reduction between threads is performed
  - Solution: when thread maximum is reset, reset for entire warp

- Each thread may load numbers of very different magnitude leading to different bin indices
  - E.g., index differs between threads in a warp
  - Not a problem on SIMT, perhaps a problem on SIMD?

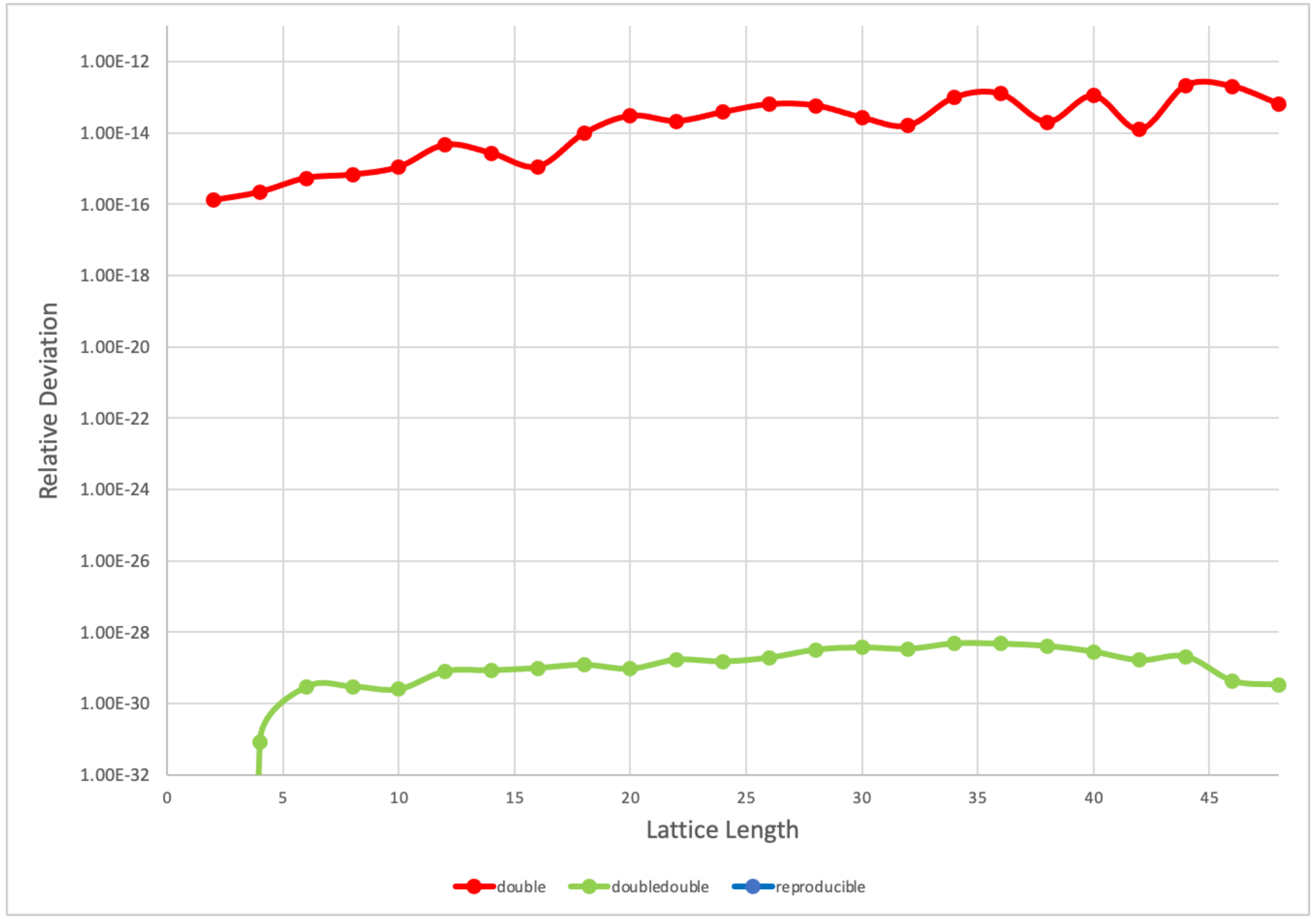
Reproducible Summations on GPUs

QUDA Implementation



Performance on Norm2 reduction kernel, fp64 inputs

(Quadro GV100, CUDA 12.1)



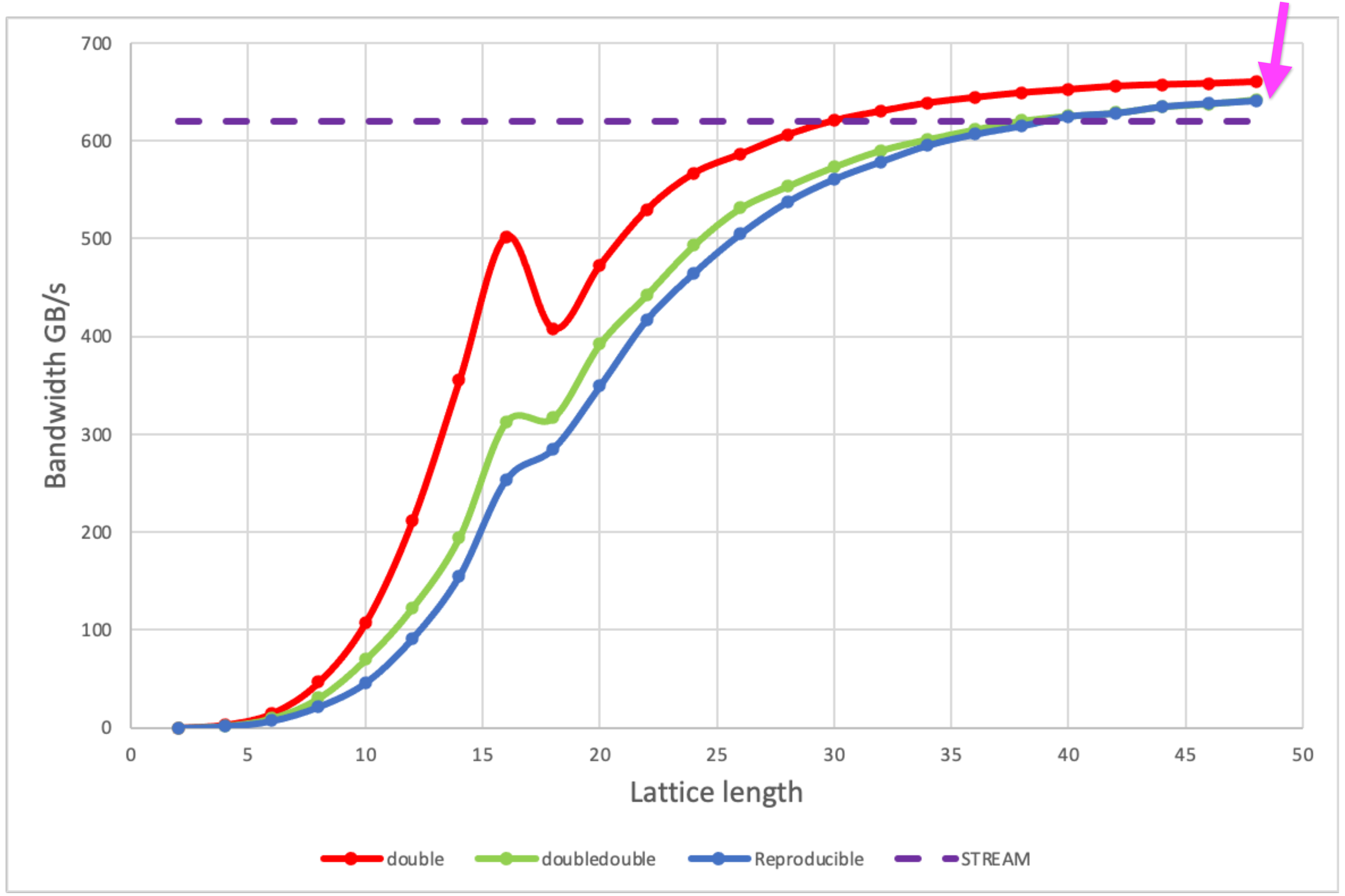
Relative Deviation between CPU and GPU Norm2 reductions

Reproducible reductions are bitwise identical as expected

Reproducible Summations on GPUs

QUDA Implementation

Aside: H100 can pull over 3 TB/s



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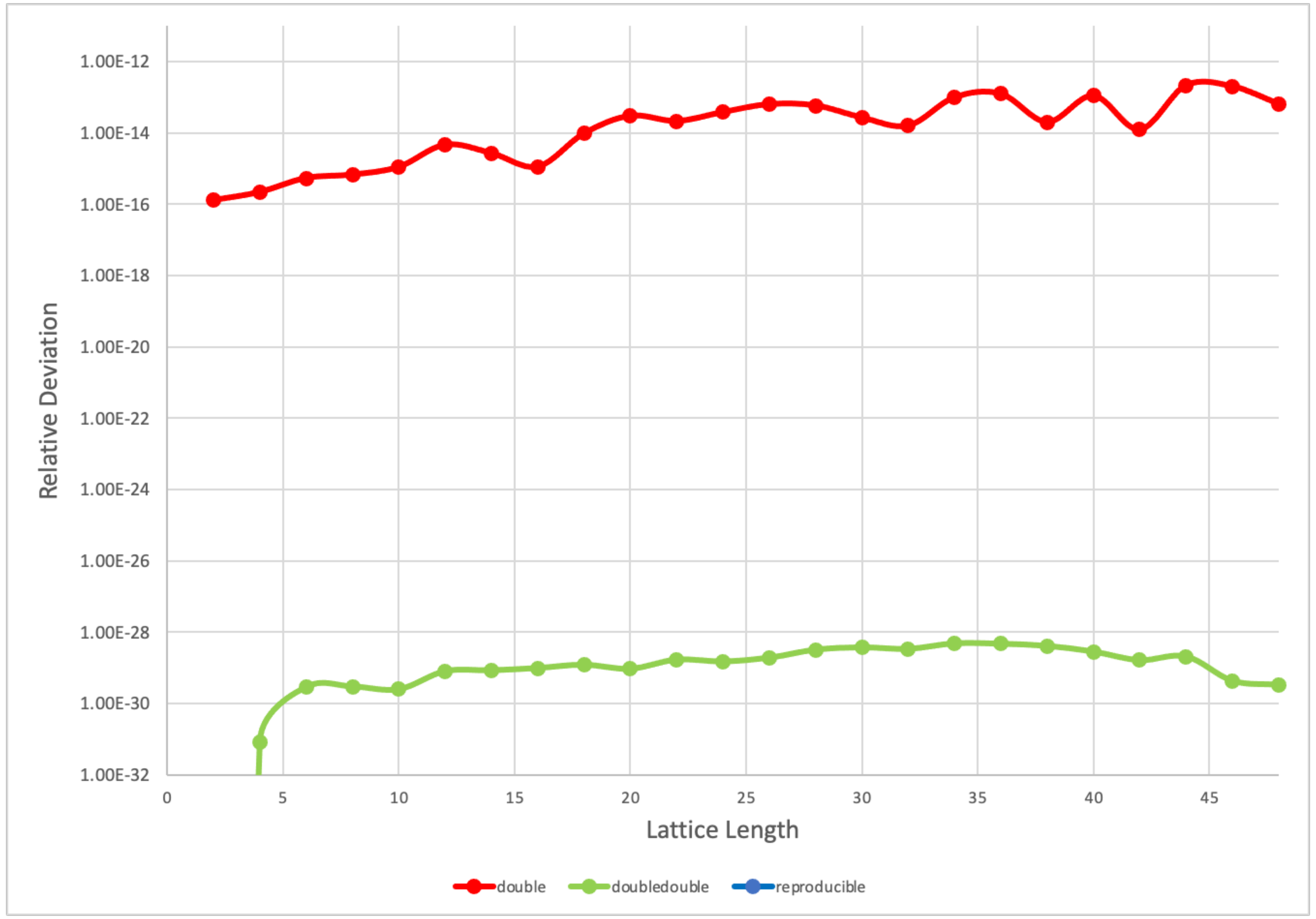

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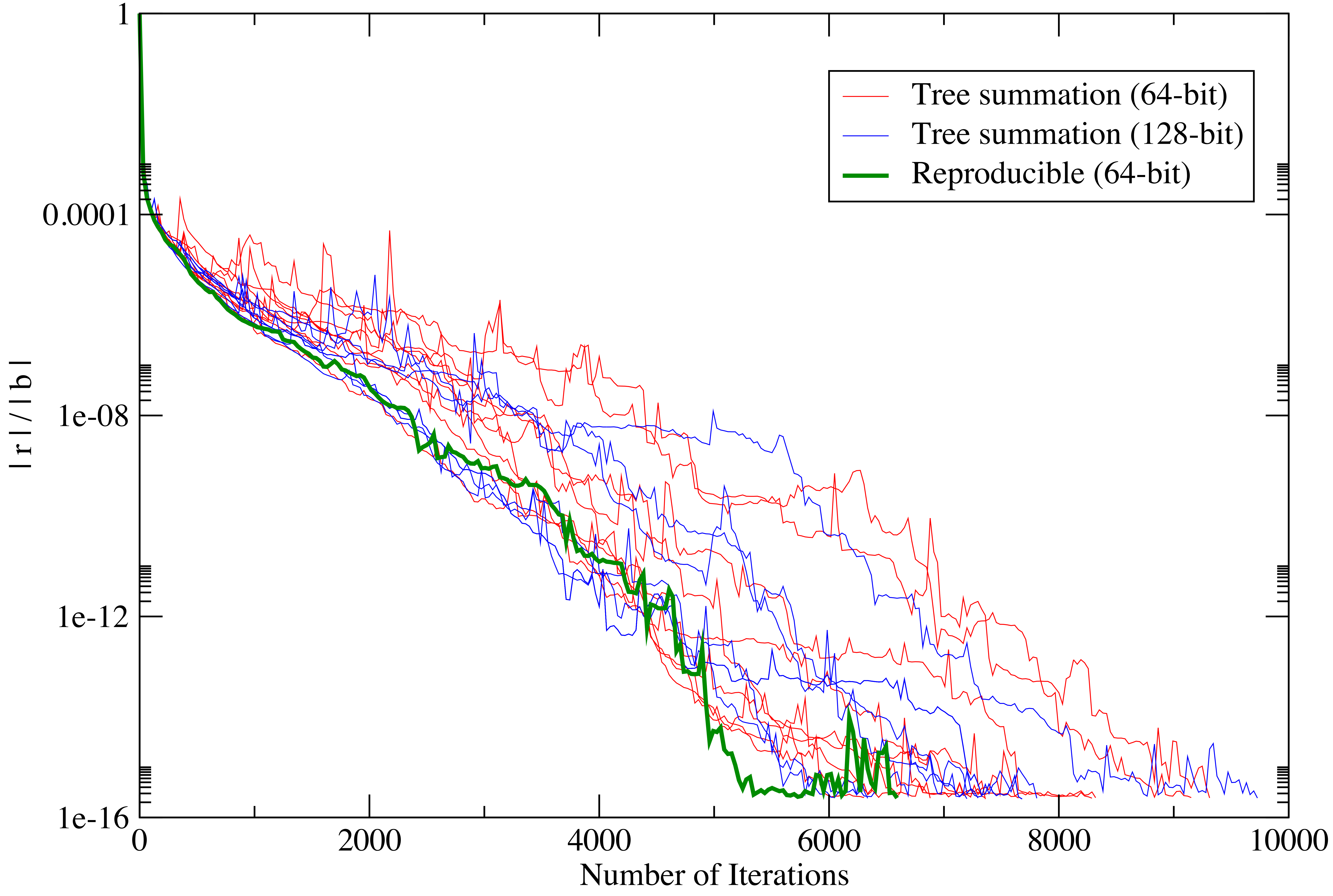
- Double-double reductions
  - 6 unique convergence histories
- Reproducible reductions
  - 1 unique convergence history



Future Work

- Add support for reproducible 128-bit summation

- Optimize
  - Partial reduction memory writing (will improve performance for intermediate sizes)
  - MPI Allreduce (presently implemented using all gather and local sum)

- Reproducible algorithm abuses floating point to behave as integers
  - Why not just use actual integers?
  - Integers have a number of advantages
    - No wasted bits for storing the exponent
    - Fewer resources required for same precision (less registers, less memory traffic)
    - NVIDIA GPUs have hardware-accelerated warp-wide integer reductions (Ampere onwards)

Summary

- Lack of floating point associativity leads to lack of reproducibility for parallel computations
- Evolved QUDA's reduction framework to allow for arbitrary reduction types and arbitrary summation algorithm
- 128-bit floating-point precision not sufficient to ensure reproducibility
- Deployed optimized reproducible reduction algorithm for bit-wise reproducible results
- Reproducibility doesn't need to cost the earth
- **Restoration of the Scientific Method**

https://github.com/lattice/quda/tree/feature/reproducible