Computational Reproducibility in Production Physics Applications

Numerical Reproducibility at Exascale Workshop
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The Problem

- Finite precision arithmetic is not associative
- Parallel global sums are non-reproducible on different numbers of processors
  - Hides programming errors
  - Can’t demonstrate that implementation conserves mass, etc. which means it is not verified and may not have the robustness properties guaranteed by the Lax-Wendroff theorem

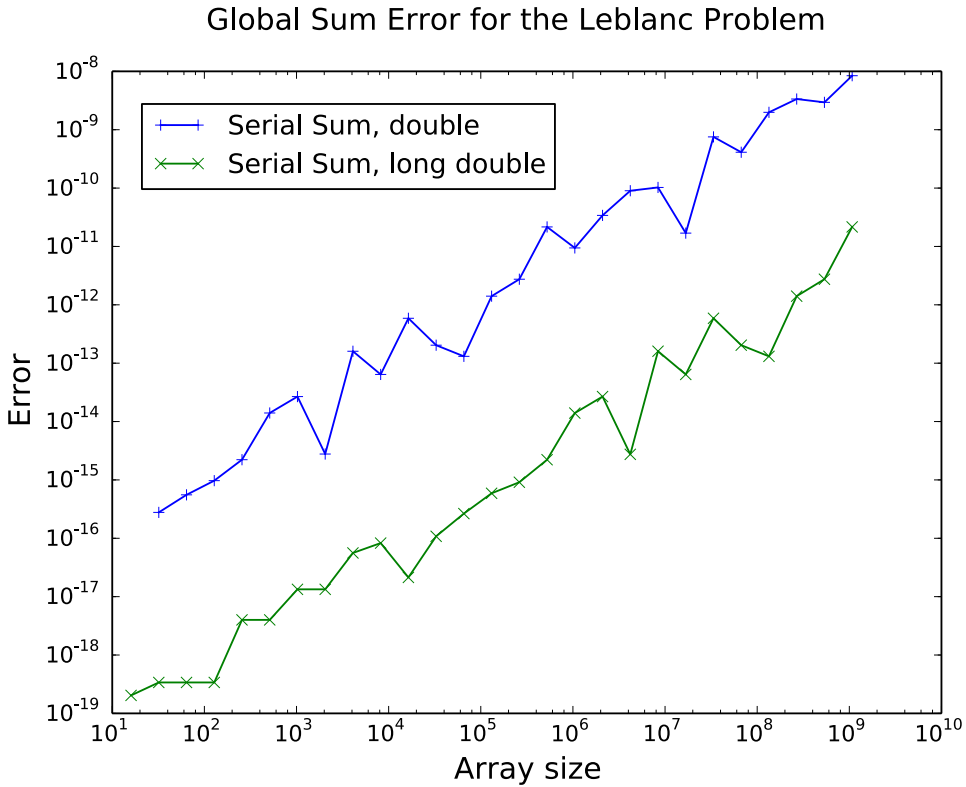
Importance at Exascale

- Predictive simulation requires improved quality of simulations
- New hardware with vectors and threads exacerbates the problem
- As size of calculations increase, the global sum error increases proportionally

Test Problem

- Leblanc's problem also known as shock tube from hell
  - 1.0e9 dynamic range in data
  - Compute sum and compare with correct sum calculated analytically

Problem grows with size



The Insight

- Reproducible global sums thought to require summation in a fixed order, but
- It can also be addressed by enhancing precision because regular addition is associative

=> Can use both enhanced precision and order to reduce precision loss

Possible Solution Components

- Enhanced precision techniques
  - Kahan sum – accumulates error on one term
  - Knuth sum – accumulates error on both terms
  - Quadtype
- Pair-wise summation
- Precision truncation
- MPI enhanced precision sum (covered in previous talks/papers)

The Results

http://www.github.com/losalamos/GlobalSums

Method	Error	Run-time (msecs)
Double	-1.99e-09	0.116
Double w/truncation	0.0	0.120
Long Double	-1.31e-13	0.118
Long Double w/truncation	0.0	0.116
Kahan Sum	0.0	0.406
Knuth Sum	0.0	0.704
Pair-wise Sum	0.0	0.402
Quad Double	5.55e-17	3.010
Full Quad Double	-4.81e-27	2.454
OpenMP double	2.465e-10	0.048
OpenMP Kahan	1.39e-16	0.063

Surprising Application

- Automatic fault recovery in a shallow-water code tracks the mass conservation and automatically restarts if it changes by more than a small amount. The quality of the global mass sum needs to be high to avoid false positives.

Open Source Playground

http://www.github.com/losalamos/GlobalSums

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