Verificarlo: tuning performance and accuracy

Pablo de Oliveira <pablo.oliveira@uvsq.fr>

SIAM CSE, March 1st 2023

LI-PaRAD, UVSQ, Université Paris-Saclay

Environmental impact of HPC

- Unprecedented climate crisis. France plans a 40% decrease in energy consumption by 2050 (increased efficiency or sobriety).

- What are the consequences for the HPC field ?
  - part of the solution: climate models, engineering improvements
  - part of the problem: energy consumption, Frontier (ORNL) consumes 21MW: the energy of a small town (16 000 french houses).
  - Optimization? improve energy efficiency in software or hardware.

Computing within planetary limits: less is more?

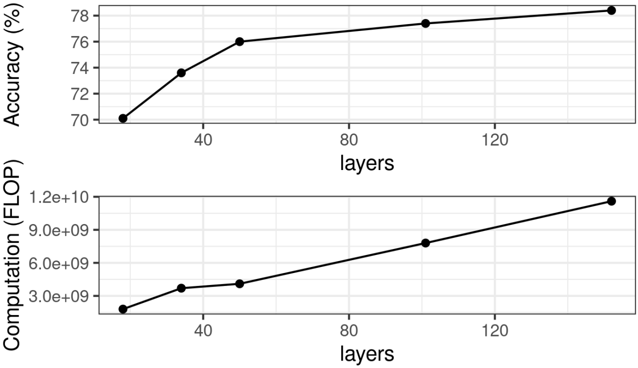
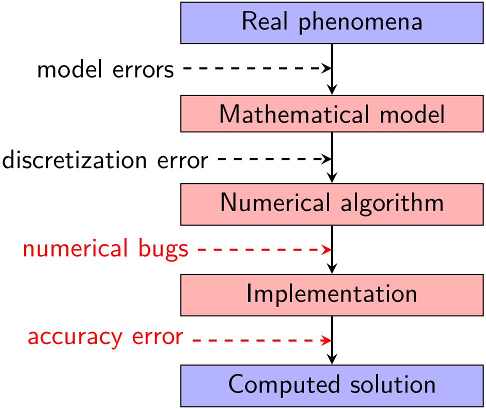


Figure: Schwartz, Green AI 2019. Resnet computation vs accuracy

- Diminishing returns: a linear increase in computation cost translates into a logarithmic accuracy gain.
- Should we compute less? Why use a large scale model when a smaller one suffices?

Numerical codes

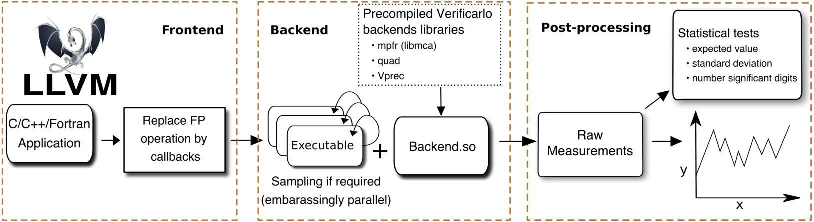


- Explore trade-offs between precision and performance
- $x = \pm 2^e \times m$
- binary64: 52 bits pseudo-mantissa
- binary32: 23 bits pseudo-mantissa

Verificarlo

Verificarlo github.com/verificarlo/verificarlo

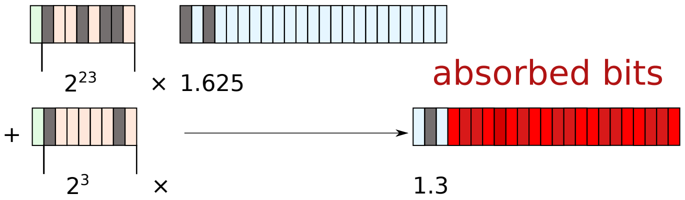
- Based on the LLVM compiler
- Active open source project with 15 contributors
- Backends: debugging (MCA, Cancellation) + mixed-precision (Vprec)
- MCA overhead from $\times 6$ (binary32) to $\times 160$ (binary64).



Verificarlo: Checking Floating Point Accuracy through Monte Carlo Arithmetic.

Denis, de Oliveira Castro, Petit. IEEE Symposium on Computer Arithmetic 2016

Floating-point arithmetic errors



IEEE-754 implementation guarantees for $\circ \in \{+, -, *, /\}$ that

$$\widehat{z} = fl(x \circ y) = (x \circ y)(1+\delta) \quad \text{with } |\delta| \leq u \text{ unit roundoff}$$

$(1+\delta)$ captures the relative error of an IEEE-754 operation

Monte Carlo Arithmetic [Stott Parker, 1999]

- Each FP operation may introduce a δ error

$$\widehat{z} = fl(x \circ y) = (x \circ y)(1 + \delta)$$

- Monte Carlo Arithmetic key principle
  - Make δ a random variable (stochastic rounding)
  - Monte Carlo sampling

- The values returned by n runs of the program using stochastic arithmetic are seen as realizations of a random variable X.
- $\hat{\mu}$ and $\hat{\sigma}$ are the empirical average and standard deviation.

Why Monte Carlo Arithmetic?

- Compare computation against an exact reference is easier.
- Sometimes,
  - hard to get an exact reference value (intermediate computations)
  - different results are not necessarily wrong

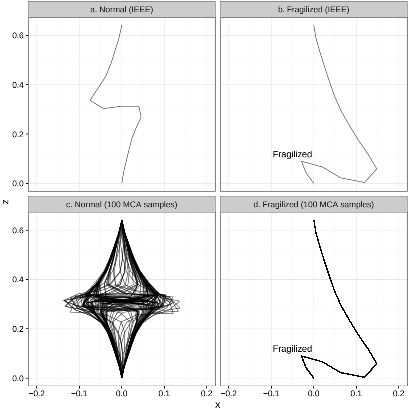


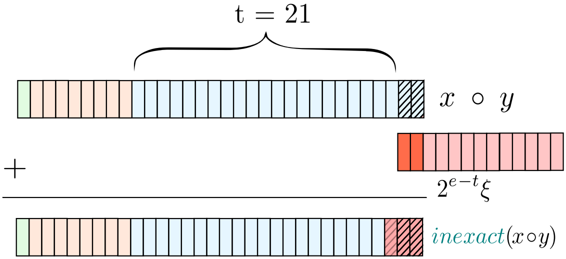
Figure: Buckling of a 1D beam with Europlexus collaboration with O. Jamond

Monte Carlo Arithmetic: Random Rounding

- MCA simulates error with

$$inexact(x) = x + 2^{e_x - t}\xi$$

  - $e_x = \lfloor \log_2 |x| \rfloor + 1$ is the order of magnitude of x;
  - ξ is an uniform random variable in $(-\frac{1}{2}, \frac{1}{2})$;
  - t is the virtual precision, selects the magnitude of the simulated error.



$$mca(x \circ y) = round(inexact(x \circ y))$$

absorption and rounding errors

Example: Linear 2x2 System

- Ill-conditioned linear system (condition number 2.5×10^8).
- We solve it with the Cramer's formula.

$$\begin{pmatrix} 0.2161 & 0.1441 \\ 1.2969 & 0.8648 \end{pmatrix} x = \begin{pmatrix} 0.1440 \\ 0.8642 \end{pmatrix}$$

$$x_{\text{real}} = \begin{pmatrix} 2 \\ -2 \end{pmatrix} \qquad x_{\mathrm{IEEE}} = \begin{pmatrix} 1.9999999958366637 \\ -1.9999999972244424 \end{pmatrix}$$

- The IEEE-754 binary64 result has 8 significant decimal digits or 28.8 significant bits.

MCA 2x2 System: Stott Parker's significant bits

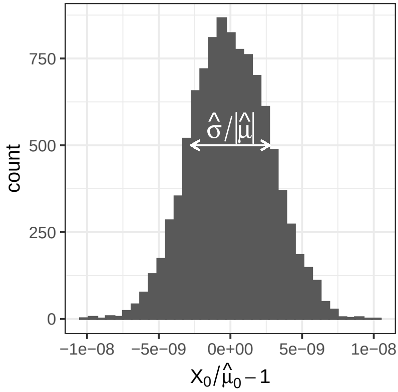


Figure: Error distribution for 10000 samples FULL MCA ($t = 53$)

$1.9999999850477848e+00$

$1.9999999957687429e+00$

$2.0000000024646973e+00$

- Stott Parker defines the number of significant bits as

$$s_{\text{PARKER}} = -\log_2 \frac{\hat{\sigma}}{|\hat{\mu}|} \approx 28.5.$$

$$(s_{\text{IEEE}} \approx 28.8)$$

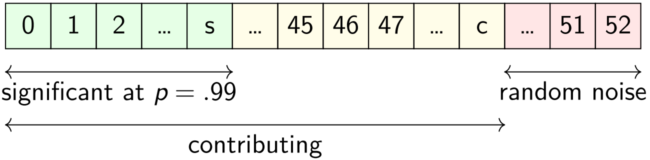
- Magnitude of the signal to noise ratio.
- But how confident are we that it is a good estimate?

Probabilistic definition of Significant bits

Significant bits

The number of significant bits with probability p can be defined as the largest number s such that

$$\mathbb{P}\left(|Z| \leq 2^{-s}\right) \geq p \quad \text{where } Z = X/X_{ref} - 1$$



Confidence Intervals for Stochastic Arithmetic. Sohier, de Oliveira Castro, Févotte, Lathuilière, Petit, Jamond. ACM Transactions Mathematical Software 2022.

CNH: Significant bits lower bound

- Given a centered normal error distribution (CNH) and $X_{ref} = \hat{\mu}$ we show

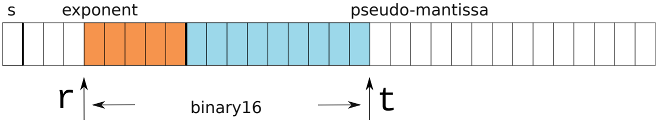
$$s \geqslant \underbrace{-\log_2\left(\frac{\hat{\sigma}}{|\hat{\mu}|}\right)}_{s_{\text{PARKER}}} - \left[\underbrace{\frac{1}{2}\log_2\left(\frac{n-1}{\chi^2_{1-\alpha/2}}\right)}_{\chi^2 \text{ confidence interval on } \hat{\sigma}} + \underbrace{\log_2\left(F^{-1}\left(\frac{p+1}{2}\right)\right)}_{\text{depends only on } p}\right] \tag{1}$$

- F is the cumulative distribution function of $\mathcal{N}(0,1)$.
- For $n \to \infty$ samples and $p = 0.68$ $s \geq -log_2\hat{\sigma}/|\hat{\mu}|$ (Parker)
- For $n = 30$ samples and $p = 0.99$ $s \geq -log_2\hat{\sigma}/|\hat{\mu}| - 1.792$
- For $n = 15$ samples and $p = 0.99$ $s \geq -log_2\hat{\sigma}/|\hat{\mu}| - 2.023$

A Bernoulli estimator provides a probabilistic lower-bound s for general distributions.

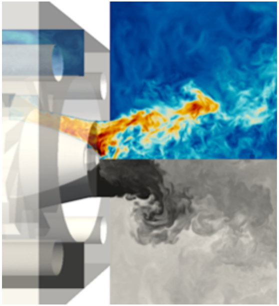
VPREC for mixed precision

- Estimate numerical effect of bfloat16, tensorflow32, fp24 on standard IEEE-754 hardware (before paying the porting cost)
- VPREC emulates any range and precision fitting in original type
  - Uses native types for storage and intermediate computations
  - Handle overflows, underflows, denormals, NaN, $\pm\infty$
  - Rounding to nearest (faithful)
  - Fast: $\times$ 2.6 to $\times$ 16.8 overhead



YALES2 application

- Computational Fluid Dynamics solver from Coria-CNRS



- Deflated Preconditioned Conjugate Gradient
- CG iterations alternate between a:
  - Deflated coarse grid
  - Fine grid

VPREC: Find minimal precision over iterations that preserves convergence (dichotomic exploration)

Automatic exploration of reduced floating-point representations in iterative methods. Chatelain, Petit, de Oliveira Castro, Lartigue, Defour. Euro-Par 2019

Mixed-precision on Yales2

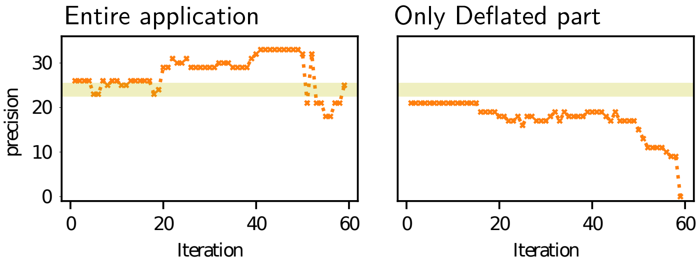


Figure: Minimal precision that preserves convergence.

Energy	16% gain on the deflated part
Communication	28% gain on communication volume
Time	10% speedup on CRIANN cluster (560 nodes)

Efficiency gains in HPC offset by increasing demand

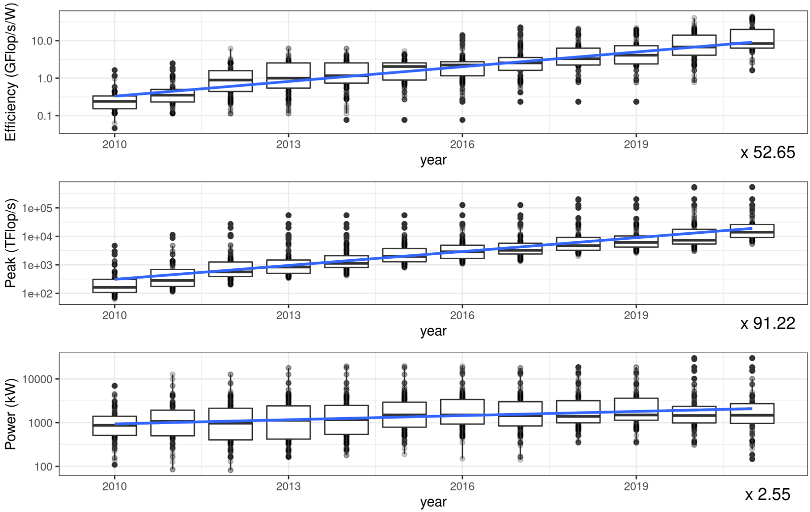


Figure: Evolution over time of the top 100 HPC systems list.

Rebound effects: direct (×2.5 average power increase) and indirect

Annex slides

Stochastic rounding can mitigate error propagation

Let us consider the inner product $y = a^\top b$ where $a, b \in \mathbb{R}^n$. We consider the forward error $Z = \frac{|\hat{y}-y|}{|y|}$.

- SR (MCA RR) errors bounds are asymptotically better

IEEE-754 in $O(n)$

$Z \leq \mathcal{K}_1 \gamma_n (u/2)^n$

SR in $O(\sqrt{n})$

- Ipsen (AH):
  $Z \leq \mathcal{K}_1 \sqrt{u\gamma_{2n}(u)}\sqrt{\ln \frac{2}{\lambda}}$
- Ours (BC):
  $Z \leq \mathcal{K}_1 \sqrt{\gamma_n(u^2)}\sqrt{\frac{1}{\lambda}}$

where $\gamma_n(u) = (1+u)^n - 1$ and K_1 is the condition number of y.

Stochastic Rounding Variance and Probabilistic Bounds: a new approach. El Arar, Sohier, de Oliveira Castro, Petit. Arxiv Preprint, July 2022.

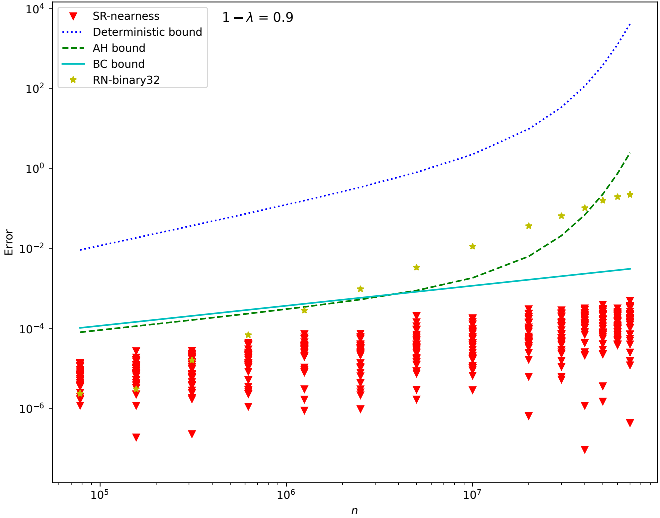


Figure: SR vs. IEEE-754 for the inner product with inputs in $(0, 1)$

- SR mitigates the biased absorptions in the IEEE-754 RN summation.
- MCA is not always a good model for IEEE-754 RN. Control divergence between MCA and RN behavior in Verificarlo studies.