Numerical Accuracy Stuff: Tools. . . and Prerequisites
Philippe Langlois

To cite this version:
Philippe Langlois. Numerical Accuracy Stuff: Tools. . . and Prerequisites. CTAOptSim General Workshop, Dec 2018, Montpellier, France. lirmm-02059798

HAL Id: lirmm-02059798
https://hal-lirmm.ccsd.cnrs.fr/lirmm-02059798
Submitted on 6 Mar 2019

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
Numerical Accuracy Stuff:
Tools... and Prerequisites

Philippe Langlois
DALI, University of Perpignan Via Domitia
LIRMM, UMR 5506 CNRS-UM, France
Blind use of tools = Hazard
Motivations

- Blind use of tools = Hazard
- FPA is an error-prone subject
- Many many recent tools … but free space towards panacea

Prerequisites

- Floating point arithmetic for dummies
- Errors and measures
- Accuracy vs. Precision: the rule of thumb
- Motto: Don’t forget the problem and its data!

Tools

- What tool for which question?
- Tools: some well-known oldies
- Tools: some works in progress
Context and motivations

Sources of errors in numerical computing

- Mathematical model
- Truncation errors
- Data uncertainties
- Rounding errors

Rounding errors may totally corrupt a FP computation

- Floating-point arithmetic approximates real one
- Accumulation of billions of floating point operations
  - May compensate...
  - but very few are enough to ruin effort
- Intrinsic difficulty to accurately solve the problem
  - Data dependency, condition
Evaluation of univariate polynomials with exact floating point coefficients

$p(x) = (x - 2)^9$ around $x = 2$ in IEEE binary64

- expanded form
Evaluation of univariate polynomials with exact floating point coefficients

\[ p(x) = (x - 2)^9 \] around \( x = 2 \) in IEEE binary64

- expanded form
- developed polynomial + Horner algorithm

Interesting example!

- Problem? No problem: exact data!
- One problem + one algorithm + one precision
  but different accuracy for different data
- Algorithms:
  - the rich vs. the poor
  - the good vs. the ugly: summation
Example: Industrial case

OpenTelemac2D simulation of Malpasset dam break (1959)

- A five year old dam break: 433 dead people and huge damage
- Triangular mesh: 26000 elements and 53000 nodes
- Water flow simulation → 35min. after break, 2sec. time step

Reproducible simulation? Accurate simulation?

<table>
<thead>
<tr>
<th></th>
<th>velocity U</th>
<th>velocity V</th>
<th>depth H</th>
</tr>
</thead>
<tbody>
<tr>
<td>The sequential run</td>
<td>0.4029747E-02</td>
<td>0.7570773E-02</td>
<td>0.3500122E-01</td>
</tr>
<tr>
<td>one 64 procs run</td>
<td>0.4935279E-02</td>
<td>0.3422730E-02</td>
<td>0.2748817E-01</td>
</tr>
<tr>
<td>one 128 procs run</td>
<td>0.4512116E-02</td>
<td>0.7545233E-02</td>
<td>0.1327634E-01</td>
</tr>
</tbody>
</table>
Bitwise reproducibility failure: gouttedo test case

time step = 2

time step = 8
1 Context and motivations

2 Prerequisite
   - FPA for dummies
   - Errors and Measures
   - Accuracy vs. Precision: The Rule of Thumb

3 Tools
   - Old Folks
     - Interval arithmetic
     - CADNA, verrou
   - Recent Tools
     - Herbgrind
     - FP Bench

4 Conclusion

5 References
IEEE-754 floating point arithmetic (1985, 2008))

Discretisation (toy system) and precision
- Normal floating point: \( x = (-1)^s \cdot m \cdot 2^e = \pm 1.x_1x_2\ldots x_{p-1} \times 2^e \)
- Precision: \( 2u = 1^+ - 1 = 2^{-p} \)

Rounding, correct rounding and unit roundoff
- \( \circ(x) = x \) for \( x \in \mathbb{F} \), else \( \circ(x) = x(1 + e) \) with \( |e| \leq u/2 \) (or \( u \))
- Correct rounding: best accuracy for \(+, -, \times, /, \sqrt{\cdot}\)
- IEEE-754
  - binary32: \( u \approx 5 \cdot 10^{-8}, p = 24, e \in \{-126 \ldots 127\} \)
  - binary64: \( u \approx 10^{-16}, p = 53, e \in \{-1022 \ldots 1023\} \)
Floating Point Arithmetic is Error Prone

### Counter intuitive FPA

- **Add is not associative**
- **Absorption**: \((1 + u) + u \neq 1 + (u + u)\)
- **Catastrophic cancellation**: \((1 + u) - 1 = 0\)
- **Order matters**: \((1 - 1) + u = u\)
- **Exact subtraction** \(x - y\) for \(1/2 \leq x/y \leq 2\) (Sterbenz)
- **Error Free Transformations (EFT)** for +, ×:
  - add: \(x + y = s + e\),
  - sub: \(x \times y = p + e\),

  everybody being *computable* FP values
Automatic Rounding Error Stuff is difficult

Track large errors?

- Small local errors may have large global effect
  - catastrophic cancellation = 1 accurate add + 1 exact sub
- Large local errors may have no global effect
  - error cancellations: \( r = (x + y) + z \) for \( x, y, z \) resp. computed by \( 1/u + 1, -(1/u + 1) \), \( u \) yields exact \( r = u \)
- Expression error depends on argument values
  - \( (x + y) + z \) is accurate except for catastrophic cancellation values

Motto: don’t forget the problem and its data!

Practical limitations: scaling and modularity effects

- Tuning \( n \) FP operations between 2 precisions = \( 2^n \) cases
- \( f(t) + z \) with accurate \( f(t) = x + y \) is accurate except for catastrophic cancellation values
Errors and Measures: A Large Array

Errors

- Forward error: $x - \hat{x}$, in the result space
- Backward error: $d - \hat{d}$, in the data space, for identified $\hat{d}$ such that $f(\hat{d}) = \hat{f}(d)$
- Absolute vs. Relative error
- Maximum vs. Average error
- Error measures: ULPs [1], bits, significant digits [4], no dimension value, interval
- Error bounds: proven vs. estimated vs. measured
Accuracy vs. Precision: The Rule of Thumb (RoT)

RoT: Accuracy $\lesssim$ Condition Number $\times u$

- Forward error $\lesssim$ condition $\times$ backward error
- Backward stable in precision $u$: relative backward error $\approx u$

Condition number

- $\lim_{\delta \to 0} \sup_{|\Delta x| \leq \delta} \frac{|\Delta y|}{|y|} / \frac{|\Delta x|}{|x|}$,
  with $y + \Delta y = f(x + \Delta x)$ and $y = f(x)$.
- Differentiable $f$: $\frac{|x||f'(x)|}{|f(x)|}$, $\frac{|x||J(x)|}{|f(x)|}$
- Motto: depends both on problem $f$ and data $x$
- Example for summation:
  - $\text{cond}(\sum_n x_i) = \sum_n |x_i| / |\sum_n x_i|$
  - Arbitrarily larger than $1/u$ when catastrophic cancellation in $\sum_n x_i$
Accuracy \preceq \text{Condition number} \times u
### How to verify or validate the accuracy of a FP computation?

- **Verify vs. validate**
- **[M]** Backward error analysis, probabilistic analysis, ad-hoc rounding error analysis
- **[T]** Interval arithmetic, stochastic arithmetic, sensitivity analysis, static analysis (+arithmetic models), dynamic analysis (+bounds, +references), formal proof assistants

### How to identify the error sources?

- **[M]** Numerical analysis vs. **Rounding error analysis**
- **[M/T]** Algorithm/Program instructions vs. **Input data range**
- **[T]** Shadow computation: random, stochastic, higher precision, EFT, “exact”, AD
How to improve the accuracy of a FP computation?

- From accurate *enough* to correctly rounded for a given precision
- [T] More hardware precision, extended precision libraries
- [M/T] More accurate algorithms: expression order, other expression, EFT
  - Hand-made vs. Automatic rewriting tools

Tools: Cost, Efficiency and Tuning

- Cost: reasonable computing time overheads for running solutions
- Efficiency: sharp vs. overestimated bound, false positive ratio, non robust optimization
- Tuning: rewrite with a minimal precision for a given accuracy
How to recover the numerical reproducibility of parallel FP computation?

- Reproducible *enough* (*i.e.* modulo validation) vs. bitwise identical
  - At least to debug parallel vs. sequential,
  - also to validate for production step, to certify for legal process
- Reproducible algorithms, libraries vs. hand-made corrections
1 Context and motivations

2 Prerequisite
- FPA for dummies
- Errors and Measures
- Accuracy vs. Precision: The Rule of Thumb

3 Tools
- Old Folks
  - Interval arithmetic
  - CADNA, verrou
- Recent Tools
  - Herbgrind
  - FP Bench

4 Conclusion

5 References
Interval Arithmetic (1966)

**IA at a glance**

- Data range or FP arithmetic $\rightarrow$ intervals + interval operation
- A sure (•) but too conservative (●) propagation of absolute errors (●)
- Dependency problem, wrapping effect, variable decorrelation, conservative inclusion of convex set; intervals containing zero
  - width([x] − [x]) = 2 width((x)),
  - tight function range: tight interval $[F([x])]$
- Best computing flow driven convex set?
  - endpoint pair, center+radius, subdivisions, Taylor expansions, affine arithmetic, zonotope, ...

\[
[x_{k+1}] = R([x_k] \text{ for } R = R(0, \pi/4) \text{ and } x_0 = [-\varepsilon, \varepsilon])
\]
Interval arithmetic

**Interval RoT [2]**

- width(f(X)) ≤ λF(X)width(X), where λF: Lipschitz-constant of f.

**Tools for Interval Arithmetic**

IntLab (Rump), MPFI (Revol) and many other
Stochastic Arithmetic

Stochastic Arithmetic (1986, 1995)

- Rounding errors are independent identically distributed (uniform) random variables (+) + (CLT) Gaussian distribution around the exact result of their global effect
- Estimation of the number of significant digits with very few values: N=3 samples are enough

Tools: Cadna (UPMC)

- Random IEEE rounding modes, synchronicity + computing zero → self validation
- Practical tool at industrial scale: languages, parallelism, support
- New stochastic numeric types + Library + source to source translator
- ×15-45 overhead: costly hardware rounding mode change

Tools: verrou (EDF)

- Parametrized random rounding modes, asynchronicity,
- ×10-20 overhead, “no” warning, post-processing tests
- Binary instrumentation (Valgrind), excluded parts (libm)
Many recent tools (2013 →)

**Proven bounds for snippets**
- Abstract model of FPA, forward error: proven (●) but conservative (●)
- Small size targets: 10-20 LOC

**Rewriting snippets**
- 10 LOC

**Detecting candidate error causes**
- Dynamic analysis (Valgrind), shadow computation: MPFR
- False positive, overhead
- Small size targets (●) ... until Herbgrind: 300K LOC (●●●)
Herbgrind (2018)

- Dynamic analysis, binaries (Valgrind)
- Large programs, different languages, libraries
- Numerical tricks detection: compensation, EFT
- Open platform: front-end to “small sized oriented tools”, ...
- Input range limitations

Steps

- Detecting FP errors: exact shadow computation (MPFR) for every FP assignation
- Collecting root cause information
  - selected error dependency chains, symbolic expression, input characteristics

Validation cases

- Gram-Schmidt Orthonormalization, PID controller
- GROMACS: molecular dynamics simulation
  - SPEC FPU, 42K LOC in C + 22K LOC in Fortan
- TRIANGLE: accurate and robust mesh generator
FPBench Project

A community infrastructure for cooperation and comparison

- FPCore: description format for FP benchmarks
- Benchmarks: suite drawn for published results
  - 111 benchs (v1.1, oct. 2018)
  - FPTaylor (CPU. Utah), Herbie (PLSE, U. Washington), Rosa (AVA, MPI-SWS, Saarbrücken), Salsa (LAMPS, UPVD)

Pros & Cons

- FPCore for fair comparison
- Small size cases, numerically safe case (worst 30% cases error = 5-6 bits)
- Others benchmarks: SPEC FPU, Hamming’s book,…
Conclusion

- Numerical accuracy stuff: large and old subject, large literature, many tools but free space for human expertise up to the ideal tools
- Our Motto = hard issue to automatic tools
- Herbgrind: a gap in recent developments?
- Corsika: tuning to low precision FP formats $\rightarrow$ full benefit of SIMD speedup e.g. $\text{AVX512} = 16 \times \text{binary32}$
Recent resources

- 30+ tools listed by M. Lam (JMU):
  https://w3.cs.jmu.edu/lam2mo/fpanalysis.html
- FPBench: http://fpbench.org,
  https://github.com/FPBench/FPBench

J.-M. Muller.
On the definition of $\text{ulp}(x)$.

A. Neumaier.
Interval Methods for Systems of Equations.

N. Revol.
Influence of the Condition Number on Interval Computations: Illustration on Some Examples.
J. Vignes.

Zéro mathématique et zéro informatique.


(In French).