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

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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
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
Example: Schoolbook level

Evaluation of univariate polynomials with exact floating point coefficients

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

- 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**

![Image 1](image1.png)

![Image 2](image2.png)

**time step = 8**

![Image 3](image3.png)

![Image 4](image4.png)
Context and motivations

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

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

Conclusion

References
Discretisation (toy system) and precision

- Normal floating point: $x = (-1)^s \cdot m \cdot 2^e = \pm 1.x_1x_2\ldots x_{p-1} \times 2^e$
  \[p \text{ bits of mantissa}\]

- 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**: $u \approx 5 \cdot 10^{-8}$, $p = 24$, $e \in \{-126\ldots127\}$
- **binary64**: $u \approx 10^{-16}$, $p = 53$, $e \in \{-1022\ldots1023\}$
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
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 \lesssim \text{Condition number} \times u

Accuracy of the polynomial evaluation \([n=50]\)

\[
\gamma_{2n} \text{ cond}
\]

\[
\begin{align*}
1e-18 & \\
1e-16 & \\
1e-14 & \\
1e-12 & \\
1e-10 & \\
1e-08 & \\
1e-06 & \\
1e-04 & \\
0.01 & 1
\end{align*}
\]

relative forward error

condition number

\(\frac{1}{u}\)
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
  - $\text{width}([x] - [x]) = 2 \text{width}((x))$
  - tight function range: tight interval $[F([x])]$
- Best computing flow driven convex set?
  - endpoint pair, center+radius, subdivisions, Taylor expansions, affine arithmetic, zonotope, ...

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

Interval RoT [2]

- width(f(X)) ≤ λ_F(X)width(X), where λ_F: 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 (\(\bullet\)) + (CLT) Gaussian distribution around the exact result (\(\bullet\)) 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 + \textit{computing zero} \rightarrow \textit{self validation}
• Practical tool at industrial scale: languages, parallelism, support
• New stochastic numeric types + Library + source to source translator
• \(\times 15-45\) overhead: costly hardware rounding mode change

Tools: verrou (EDF)

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

<table>
<thead>
<tr>
<th>Proven bounds for snippets</th>
</tr>
</thead>
<tbody>
<tr>
<td>- Abstract model of FPA, forward error: proven (●) but conservative (●)</td>
</tr>
<tr>
<td>- Small size targets: <strong>10-20 LOC</strong></td>
</tr>
</tbody>
</table>

<table>
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<tr>
<td>- <strong>10 LOC</strong></td>
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<table>
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<tr>
<th>Detecting <em>candidate</em> error causes</th>
</tr>
</thead>
<tbody>
<tr>
<td>- Dynamic analysis (Valgrind), shadow computation: MPFR</td>
</tr>
<tr>
<td>- False positive, overhead</td>
</tr>
<tr>
<td>- Small size targets (●) ... until Herbgrind: <strong>300K LOC (●●●)</strong></td>
</tr>
</tbody>
</table>
Herbgrind (2018)

- Dynamic analysis, binaries (Valgring)
- 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
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,...
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 → full benefit of SIMD speedup e.g. . AVX512 = 16 × 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 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).