Numerical Accuracy Stuff: Tools. . . and Prerequisites

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CTAOptSim General Workshop, Montpellier, dec. 6-7th, 2018

Numerical Accuracy Stuff: Tools. . . and Prerequisites

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Blind use of tools = Hazard

Lineup

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

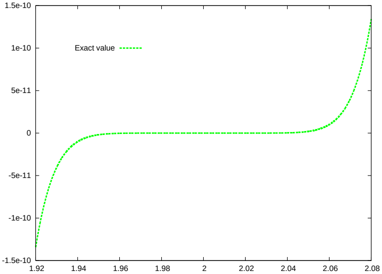
- Mathematical model
- Truncation errors
- Data uncertainties
- Rounding errors

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

Example: Schoolbook level

Evaluation of univariate polynomials with exact floating point coefficients

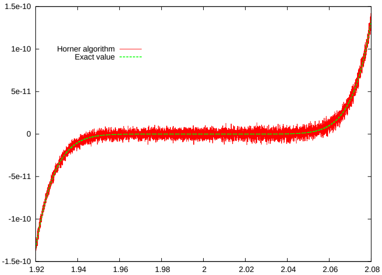


$p(x) = (x-2)^9$ around $x = 2$ in IEEE binary64

- expanded form

Example: Schoolbook level

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

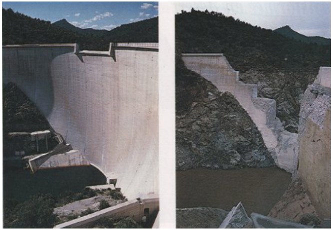
Interesting example!

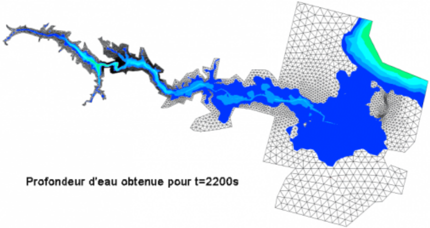
- Problem? No problem: exact data!
- One problem + one algorithm + one precision
  but different accuracy for different data
- Algorithms:
  - the rich vs. the poor
  - the good vs. the ugly: summation

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



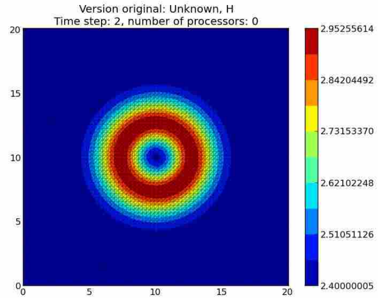


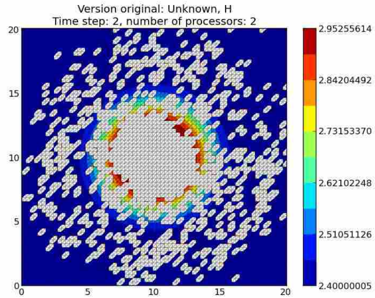
Reproducible simulation? Accurate simulation?

	velocity U	velocity V	depth H
The sequential run	0.4029747E-02	0.7570773E-02	0.3500122E-01
one 64 procs run	0.4935279E-02	0.3422730E-02	0.2748817E-01
one 128 procs run	0.4512116E-02	0.7545233E-02	0.1327634E-01

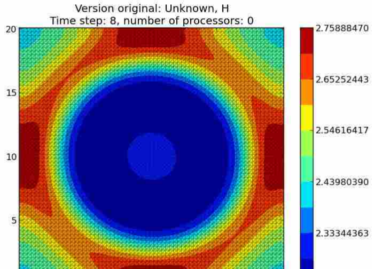
Bitwise reproducibility failure: gouttedo test case

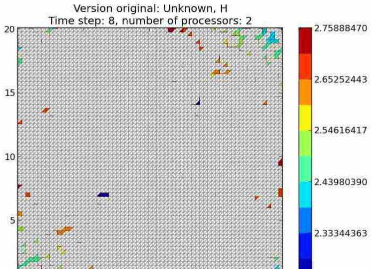
time step = 2





time step = 8





Menu

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

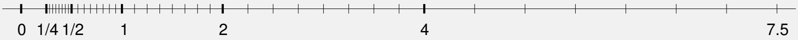
4 Conclusion

5 References

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

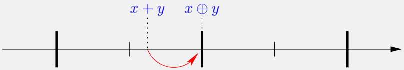
Discretisation (toy system) and precision

- Normal floating point: $x = (-1)^s \cdot m \cdot 2^e = \pm \underbrace{1.x_1 x_2 \ldots x_{p-1}}_{p \text{ bits of mantissa}} \times 2^e$
- Precision: $2\mathbf{u} = 1^+ - 1 = 2^{-p}$



Rounding, correct rounding and unit roundoff

- $\circ(x) = x$ for $x \in \mathbb{F}$, else $\circ(x) = x(1+e)$ with $|e| \leq \mathbf{u}/2$ (or $\mathbf{u}$)
- Correct rounding: best accuracy for $+, -, \times, /, \sqrt{\ }$



- IEEE-754
  - binary32: $\mathbf{u} \approx 5 \cdot 10^{-8}$, $p = 24$, $e \in \{-126 \ldots 127\}$
  - binary64: $\mathbf{u} \approx 10^{-16}$, $p = 53$, $e \in \{-1022 \ldots 1023\}$

Floating Point Arithmetic is Error Prone

Counter intuitive FPA

- Add is not associative •
- Absorption: • $(1 + \mathbf{u}) + \mathbf{u} \neq 1 + (\mathbf{u} + \mathbf{u})$ •
- Catastrophic cancellation: $(1 + \mathbf{u}) - 1 = 0$ •
- Order matters: • $(1 - 1) + \mathbf{u} = \mathbf{u}$ •
- Exact subtraction $x - y$ for $1/2 \leq x/y \leq 2$ • (Sterbenz)
- Error Free Transformations (EFT) for $+$, $\times$:
  - 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 $1/\mathbf{u} + 1$, $-(1/\mathbf{u} + 1)$, $\mathbf{u}$ yields exact $r = \mathbf{u}$
- 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: $x - \widehat{x}$, in the result space
- Backward error: $d - \widehat{d}$, in the data space, for identified $\widehat{d}$ such that $f(\widehat{d}) = \widehat{f}(d)$
- 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)

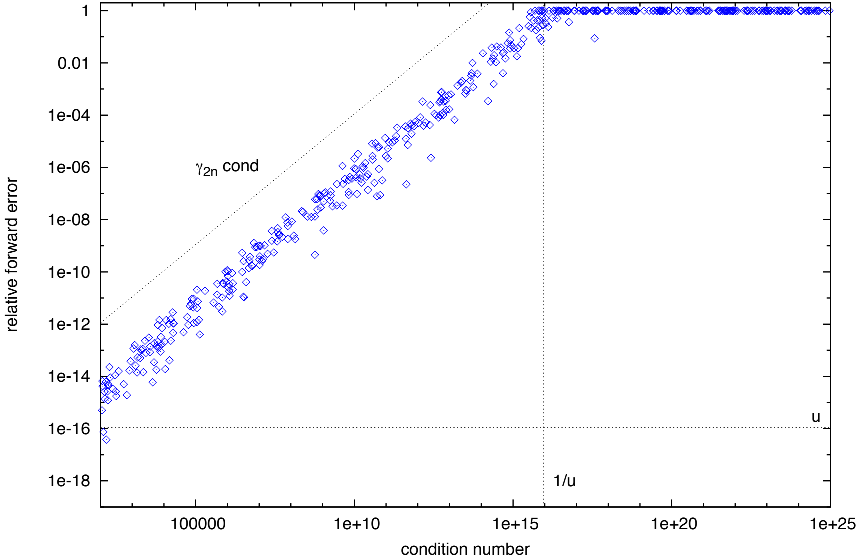
RoT: Accuracy $\lesssim$ Condition Number $\times \mathbf{u}$

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

Condition number

- $\lim_{\delta \to 0} \sup_{|\Delta x| \le \delta} \frac{|\Delta y|}{|y|} / \frac{|\Delta x|}{|x|}$,
  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 $1/\mathbf{u}$ when catastrophic cancellation in $\sum_n x_i$

Accuracy $\lesssim$ Condition number $\times \mathbf{u}$



Numerical Accuracy Stuff: Aims, Methods and Tools I

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

Numerical Accuracy Stuff: Aims, Methods and Tools II

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

Numerical Accuracy Stuff: Aims, Methods and Tools III

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

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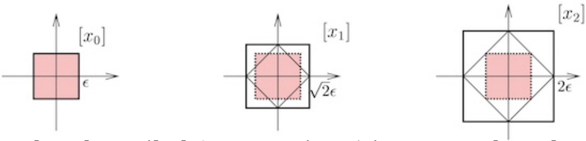
Interval Arithmetic (1966)

IA at a glance

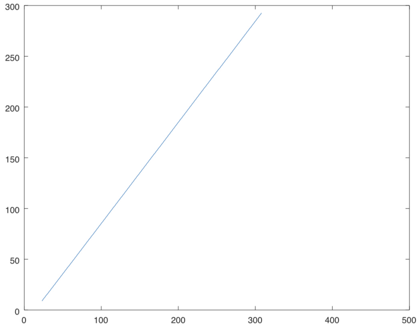
- Data range or FP arithmetic $\rightarrow$ intervals + interval operation
- A sure (•) but too conservative (•) propagation of absolute errors (•)
- Dependency problem, wrapping effect, variable decorrelation, conservative inclusion of convex set; intervals containing zero
  - width$([x] - [x]) = 2$ 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, ...



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

Interval RoT [2]

- $\text{width}(f(X)) \leq \lambda_F(X)\text{width}(X)$, where λ_f: Lipschitz-constant of f.



Interval sum: $\log_{10}\text{width}(s_n)$ vs. $\log_{10}\text{cond}(s_n)$ for $s_n = 1$ [3]

Tools for Interval Arithmetic

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

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 $\rightarrow$)

Proven bounds for snippets

- Fluctuat (2005, 2013), FPTaylor (2015), Rosa/Daisy (2014,2017), ...
- Abstract model of FPA, forward error: proven (•) but conservative (•)
- Small size targets: 10-20 LOC

Rewriting snippets

- Herbie (2015), Salsa (2015)
- 10 LOC

Detecting *candidate* error causes

- FPDebug (2011), Herbgrind (2018)
- Dynamic analysis (Valgrind), shadow computation: MPFR
- False positive, overhead
- Small size targets (•) . . . until Herbgrind: 300K LOC (•••)

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

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.* . AVX512 = 16 $\times$ binary32

Recent resources

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

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