Numerical validation using stochastic arithmetic

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LIP6

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- Floating-point arithmetic: the IEEE 754 standard
- The CESTAC method and the stochastic arithmetic
- The CADNA software
- Contributions of CADNA in numerical methods
- Precision autotuning

In a floating-point arithmetic using the radix *b*,

$$X = \varepsilon M b^{E}$$

is represented by:

- its sign ε, encoded on one digit (0 if X is positive, 1 if X is negative),
- its exponent E, a k digit integer,
- its mantissa *M*, encoded on *p* digits.

$$M = \sum_{i=0}^{p-1} a_i b^{-i}$$
 and $a_i \in \{0, ..., b-1\}$.

Floating-point numbers are usually normalized: $a_0 \neq 0, M \in [1, b)$ and zero has a special representation. Formats using the radix 2:

- binary16 (half precision)
- binary32 (single precision)
- *binary64* (double precision)
- *binary128* (quadruple precision)
- binary256 (octuple precision)

Formats using the radix 10 (emulate decimal rounding exactly):

- decimal32 (storage on 32 bits)
- decimal64 (storage on 64 bits)
- decimal128 (storage on 128 bits)

IEEE 754 single precision:

| 1 | 2 9 | 10 | 32 |
|---|------------------------|-----------------------|----------------------------|
| S | E + 2 ⁷ – 1 | <i>a</i> ₁ | <i>a</i> ₂₃ |

 \Rightarrow range: 10^{±38}, accuracy: $u = 2^{-24} \approx 6 \ 10^{-8}$

IEEE 754 double precision:

| 1 | 2 12 | 13 | 64 |
|---|-------------------------|------------|-----------------|
| S | E + 2 ¹⁰ – 1 | <i>a</i> 1 | a 52 |

 \Rightarrow range: 10^{±308}, accuracy: $u = 2^{-53} \approx 1 \ 10^{-16}$

Remark: $a_0 = 1$ (hidden bit)

binary16 (fp16):

- 11 bits for the mantissa, 5 for the exponent ⇒ range: 10^{±5}, accuracy: u = 2⁻¹¹ ≈ 5 10⁻⁴
- used by NVIDIA GPUs, AMD Radeon Instinct MI25 GPU, ARM NEON, Fujitsu A64FX ARM

bfloat16:

- 8 bits for the mantissa, also 8 for the exponent \Rightarrow range: $10^{\pm 38}$, accuracy: $u = 2^{-8} \approx 4 \ 10^{-3}$
- used by Google TPU, NVIDIA GPUs, ARM, Intel.

 \mathbb{F} : set of real numbers which can be coded exactly on a computer (set of floating point numbers)

Every real number $x \notin \mathbb{F}$ is approximated by a number $X \in \mathbb{F}$.

Let X_{min} (resp. X_{max}) be the smallest (resp. the greatest) floating point number:

$$\forall x \in]X_{min}, X_{max}[, \exists \{X^-, X^+\} \in \mathbb{F}^2$$

such that

$$X^- < x < X^+$$
 and $]X^-, X^+[\cap \mathbb{F} = \emptyset$



The rounding mode is the algorithm that, according to *x*, gives X^- or X^+ .

The 4 rounding modes of the IEEE 754 standard



Rounding to zero: *x* is represented by the floating point number the nearest to *x* between *x* and 0.

Rounding to nearest: *x* is represented by the floating point number the nearest to *x*.

Rounding to $+\infty$: *x* is represented by X^+ .

Rounding to $-\infty$: *x* is represented by *X*⁻.

The rounding operation is performed after each assignment and after every elementary arithmetic operation.

$$0.3 * x^2 + 2.1 * x + 3.675 = 0$$

Rounding to nearest

d = -3.81470E-06 There are two conjugate complex roots. z1 = -.3500000E+01 + i * 0.9765625E-03 z2 = -.3500000E+01 + i * -.9765625E-03

Rounding to zero

d = 0.

The discriminant is null.

The double real root is -.3500000E+01

$$0.3 * x^2 + 2.1 * x + 3.675 = 0$$

• Rounding to $+\infty$ d = 3.81470E-06 There are two different real roots. x1 = -.3500977E+01 x2 = -.3499024E+01

Sounding to −∞

d = 0.

The discriminant is null.

The double real root is -.3500000E+01

Inconsistency of the floating point arithmetic

On a computer, arithmetic operators are only approximations.

- commutativity: $X \bigcirc Y = Y \bigcirc X$
- no associativity: $(X \odot Y) \odot Z \neq X \odot (Y \odot Z)$
- no distributivity: $X \otimes (Y \oplus Z) \neq (X \otimes Y) \oplus (X \otimes Z)$

On a computer, order relationships are used as in mathematics \implies it leads to a global inconsistent behaviour.

Let *x*, *y* be exact results and *X*, *Y* the associated floating-point numbers:

$$X = Y \Rightarrow x = y$$
 and $x = y \Rightarrow X = Y$.
 $X \ge Y \Rightarrow x \ge y$ and $x \ge y \Rightarrow X \ge Y$.

Round-off error model

 $r \in \mathbb{R}$: exact result of *n* elementary arithmetic operations.

On a computer, one obtains $R \in \mathbb{F}$ which is affected by round-off errors.

R can be modeled, at the first order with respect to 2^{-p} , by

$$m{R} pprox m{r} + \sum_{i=1}^n m{g}_i(m{d}) \ 2^{-p} \ lpha_i$$

- p is the number of bits including the hidden bit
- $g_i(d)$ are coefficients depending on data and on the algorithm
- α_i are the round-off errors.

Remarks:

- the number of terms may be > n (ex: for n = 1, we have 3 terms if data are not exactly encoded)
- we have assumed that exponents and signs of intermediate results do not depend on α_i.

The number of significant bits in common between R and r is

$$C_R = -\log_2 \left| \frac{R-r}{r} \right| \approx p - \log_2 \left| \sum_{i=1}^n g_i(d) \cdot \frac{\alpha_i}{r} \right|$$

The last part corresponds to the accuracy lost in the computation of R, we can note that it is independent of p.

Theorem

The loss of accuracy during a numerical computation is independent of the precision used for the floating point representation.

Several approaches

• Inverse analysis

based on the "Wilkinson principle": the computed solution is assumed to be the exact solution of a nearby problem

- provides error bounds for the computed results
- Interval arithmetic

The result of an operation between two intervals contains all values obtained by performing this operation on elements from each interval.

- guaranteed bounds for each computed result
- the error may be overestimated
- specific algorithms

Static analysis

- no execution, rigorous analysis, all possible input values taken into account
- not suited to large programs

Probabilistic approach

- uses a random rounding mode
- estimates the number of correct digits of any computed result

The CESTAC method (Contrôle et Estimation Stochastique des Arrondis de Calculs) was proposed by M. La Porte and J. Vignes in 1974.

It consists in performing the same computation several times with different round-off error propagations. Then, different results are obtained.

Briefly, the part that is common to the different results is assumed to be correct and the part that is different is affected by round-off errors. Let *r* be the exact result of an arithmetic operation: $R^{-} \le r \le R^{+}$.



The random rounding mode consists in rounding *r* to $-\infty$ or $+\infty$ with the probability 0.5.

If round-off errors affect a result, one obtains for N different runs, N different results on which a statistical test may be applied.

By running N times a code with the random arithmetic, one obtains an N-sample of the random variable modeled by

$$R \approx r + \sum_{i=1}^{n} g_i(d) 2^{-p} \alpha_i$$

where the α_i 's are modeled by independent identically distributed random variables. The common distribution of the α_i is uniform on [-1, +1].

- \Rightarrow the mathematical expectation of *R* is the mathematical result *r*,
- \Rightarrow the distribution of *R* is a quasi-Gaussian distribution.

We use the classical Student's test which provides a confidence interval of the expectation of a Gaussian distribution from a sample.

 $\forall \beta \in [0, 1], \exists \tau_{\beta} \in \mathbb{R}$ such that

$$P\left(r \in \left[\overline{R} - \frac{\tau_{\beta} \sigma}{\sqrt{N}}, \overline{R} + \frac{\tau_{\beta} \sigma}{\sqrt{N}}\right]\right) = P\left(\left|\overline{R} - r\right| \le \frac{\tau_{\beta} \sigma}{\sqrt{N}}\right) = \beta$$

with



The relative error on \overline{R} is $\left|\frac{\overline{R}-r}{r}\right| = 10^{-C_{\overline{R}}}$

With a probability β , the number of exact significant digits of \overline{R}

$$C_{\overline{R}} \approx \log_{10} \left| \frac{\overline{R}}{\overline{R} - r} \right| \geq \log_{10} \left(\frac{\sqrt{N} \left| \overline{R} \right|}{\sigma \tau_{\beta}} \right).$$

With a probability β , the number of exact significant digits of \overline{R} $C_{\overline{R}} \approx \log_{10} \left| \frac{\overline{R}}{\overline{R}-r} \right|$ is undervalued by

$$C_{\overline{R}} \approx \log_{10}\left(\frac{\sqrt{N}|\overline{R}|}{\sigma\tau_{\beta}}\right).$$

Implementation of the CESTAC method

The implementation of the CESTAC method in a code providing a result *R* consists in:

- performing *N* times this code with the random rounding mode to obtain *N* samples *R_i* of *R*,
- choosing as the computed result the mean value \overline{R} of R_i , i = 1, ..., N,
- estimating the number of correct decimal digits of \overline{R} with

$$C_{\overline{R}} \approx \log_{10} \left(\frac{\sqrt{N} \left| \overline{R} \right|}{\sigma \tau_{\beta}} \right)$$

where

$$\overline{R} = \frac{1}{N} \sum_{i=1}^{N} R_i$$
 and $\sigma^2 = \frac{1}{N-1} \sum_{i=1}^{N} (R_i - \overline{R})^2$.

 τ_{β} is the value of Student's distribution for N - 1 degrees of freedom and a probability level β .



• each operation executed N = 3 times with a random rounding mode



- each operation executed N = 3 times with a random rounding mode
- number of correct digits in the result estimated using Student's test with the confidence level 95%

2 or 3 runs are enough. To increase the number of runs is not necessary.

From the model, to increase by 1 the number of correct digits given by $C_{\overline{R}}$, we need to multiply the sample size by 100.

Such an increase of N will only point out the limit of the model and its error without really improving the quality of the estimation.

It has been shown that N = 3 is the optimal value.

On the probability of the confidence interval

Probability of **overestimating** the number of correct digits of at least 1:

$$P\left(\log_{10}\left(\frac{\sqrt{N}\left|\overline{R}\right|}{\sigma\tau_{\beta}}\right) \ge \log_{10}\left|\frac{\overline{R}}{\overline{R}-r}\right| + 1\right)$$
$$= P\left(\frac{\sqrt{N}\left|\overline{R}\right|}{\sigma\tau_{\beta}} \ge \left|\frac{10\overline{R}}{\overline{R}-r}\right|\right)$$
$$= P\left(\left|\frac{\overline{R}}{\overline{R}-r}\right| \le \frac{\sqrt{N}\left|\overline{R}\right|}{10\sigma\tau_{\beta}}\right)$$
$$= P\left(\left|\overline{R}-r\right| \ge \frac{10\sigma\tau_{\beta}}{\sqrt{N}}\right)$$

With $\beta = 0.95$ and N = 3, the probability of overestimating the number of correct digits of at least 1 is 0.054%



Probability of underestimating the number of correct digits of at least 1:

$$P\left(\log_{10}\left(\frac{\sqrt{N}\left|\overline{R}\right|}{\sigma\tau_{\beta}}\right) \le \log_{10}\left|\frac{\overline{R}}{\overline{R}-r}\right| - 1\right)$$
$$= P\left(\frac{\sqrt{N}\left|\overline{R}\right|}{\sigma\tau_{\beta}} \le \left|\frac{\overline{R}}{10(\overline{R}-r)}\right|\right)$$
$$= P\left(\left|\frac{\overline{R}}{\overline{R}-r}\right| \ge \frac{10\sqrt{N}\left|\overline{R}\right|}{\sigma\tau_{\beta}}\right)$$
$$= P\left(\left|\overline{R}-r\right| \le \frac{\sigma\tau_{\beta}}{10\sqrt{N}}\right)$$

With $\beta = 0.95$ and N = 3, the probability of underestimating the number of correct digits of at least 1 is 29%.



By choosing a confidence interval at 95%, we prefer to guarantee a minimal number of correct digits with a high probability (0.99946), even if we are often pessimistic by 1 digit.

The CESTAC method is based on a 1st order model.

- A multiplication of two insignificant results
- or a division by an insignificant result

may invalidate the 1st order approximation.

Therefore the CESTAC method requires a dynamical control of multiplications and divisions, during the execution of the code.

The problem of stopping criteria

Let us consider a general iterative algorithm: $U_{n+1} = F(U_n)$.

```
while (fabs(X-Y) > EPSILON) {
    X = Y;
    Y = F(X);
}
```

 ε too low \implies risk of infinite loop ε too high \implies too early termination.

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}
```

 ε too low \implies risk of infinite loop ε too high \implies too early termination.

It would be optimal to stop when X - Y is an **insignificant value**.

Such a stopping criterion

- would enable one to develop new numerical algorithms
- is possible thanks to the concept of *computational zero*.

J. Vignes, 1986

Definition

A result *R* obtained using the CESTAC method is a computational zero, denoted by @.0, if

$$\forall i, R_i = 0 \text{ or } C_{\overline{R}} \leq 0.$$

This means that 0 belongs to the confidence interval.

It means that R is a computed result which, because of round-off errors, cannot be distinguished from 0.

Definition

Let X and Y be two results computed using the CESTAC method (N-samples).

• X is stochastically equal to Y, noted X = Y, iff

$$X-Y=@.0.$$

• X is stochastically strictly greater than Y, noted X s> Y, iff

$$\overline{X} > \overline{Y}$$
 and $X s \neq Y$

• X is stochastically greater than or equal to Y, noted $X \ge Y$, iff

$$\overline{X} \ge \overline{Y}$$
 or $X s = Y$

Ex: if X - Y is numerical noise, X > Y is false, but X > Y is true.

Discrete Stochastic Arithmetic (DSA) is the joint use of the CESTAC method, the computed zero and the stochastic relations.

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- $x = 0 \Rightarrow X = @.0$.
- $X s \neq Y \Rightarrow x \neq y$.
- $X \gg Y \Rightarrow x > y$.
- $x \ge y \Rightarrow X s \ge Y$.
- The relation *s*> is transitive: Xs > Y and $Ys > Z \Rightarrow Xs > Z$.
- The relation s= is reflexive: Xs = Xsymmetric: $Xs = Y \Rightarrow Ys = X$ but not transitive: Xs = Y and $Ys = Z \Rightarrow Xs = Z$ (ex : X=2.1, Y=2., Z=2.4)
- The relation s≥ is reflexive: Xs≥ X antisymmetric: Xs≥ Y and Ys≥ X ⇒ Xs= Y but not transitive: Xs≥ Y and Ys≥ Z ⇒ Xs≥ Z (ex : X=2.1, Y=@.0, Z=2.2)



The CADNA library allows one to estimate round-off error propagation in any scientific program.

CADNA enables one to:

- estimate the numerical quality of any result
- control branching statements
- perform a dynamic numerical debugging
- take into account uncertainty on data.

CADNA is a library which can be used with Fortran, C, or C++ programs and also with parallel programs (using MPI, OpenMP, CUDA).

CADNA can be downloaded from http://cadna.lip6.fr

CADNA implements Discrete Stochastic Arithmetic

CADNA provides new numerical types, the stochastic types (3 floating point variables x, y, z and an integer variable accurracy):

- half_st in half precision
- float_st in single precision
- double_st in double precision

All operators and mathematical functions are redefined for these types.

The cost of CADNA is about:

- 4 for memory
- 10 for run time.

Numerical debugging

The following instabilities can be detected:

- unstable division: the divisor is insignificant
- unstable power function: one operand of the pow function is insignificant
- unstable multiplication: both operands are insignificant
- **unstable branching**: the difference between the two operands is insignificant. The chosen branching statement is associated with the equality.
- **unstable mathematical function**: in the log, sqrt or exp function, the argument is insignificant.

unstable intrinsic function:

- inherited from Fortran
- in the floor or ceil function: the floor (or ceil) function returns different values for each component.
- in the abs function: different components have different signs.
- unstable cancellation: for addition (and subtraction)

 $\min(accuracy(a), accuracy(b)) - accuracy(a+b) > CANCEL_LEVEL$
The use of the CADNA library involves at most 6 steps:

- inclusion of the CADNA header for the compiler,
- initialization of the CADNA library,
- substitution of the classic floating-point types by stochastic types in variable declarations,
- possible changes in the input data if perturbation is desired, to take into account uncertainty in initial values,
- change of output statements to print stochastic results with their accuracy,
- termination of the CADNA library.

The **#include** <cadna.h> preprocessor directive must take place before any declaration of stochastic variables, for stochastic types and overloaded or new functions to be found by the compiler. The call to the cadna_init function must be added just after the main function declaration statements to initialize the library.

- numb_instability = -1: all the instabilities will be detected
- numb_instability = 0: no instability will be detected
- numb_instability = M (strictly positive M): the first M instabilities will be detected.

The other arguments are optional.

cadna_instability: describes which instabilities are disabled

- CADNA_DIV, CADNA_MUL, CADNA_POWER
- CADNA_BRANCHING
- CADNA_CANCEL
- CADNA_MATH, CADNA_INTRINSIC
- CADNA_ALL

cancel_level: a cancellation is detected if the accuracy difference between the two operands and the result is > cancel_level. Default: 4.

init_random: seed of the random generator used by CADNA.

The call to the cadna_end function should be the last statement.

The cadna_end function writes on the standard output a numerical stability report.

To control the numerical quality of a variable, just replace its standard type by the associated stochastic type.

| half | \Rightarrow | half_st |
|--------|---------------|-----------|
| float | \Rightarrow | float_st |
| double | \Rightarrow | double_st |

Example:

float_st a,b,c; double_st e,f,g; float_st d[6]; Before printing each stochastic variable, it must be transformed into a string by the strp function. This function returns a char \star , therefore formats in print functions should be modified.

| Initial C/C++ | Modified statements | | |
|-------------------------|---|--|--|
| code | for CADNA | | |
| float x; | <pre>#include <cadna.h> float_st x; cadna_init(-1);</cadna.h></pre> | | |
| | | | |
| nrintf("%f8 3\n" v). | printf("%s\n" strp(r)). | | |
| princi (210.3/11 , X); | princi (%S (n , Scip(x)); | | |

Changes in printing statements(2)

With the strp function, only the exact significant digits are printed. If a result has no exact significant digit, @.0 is printed.

Example:

- U(3) = 0.55901639344262E+001 U(4) = 0.5633431085044E+001 U(5) = 0.56746486205E+001 U(6) = 0.5713329052E+001 U(7) = 0.574912092E+001 U(8) = 0.57818109E+001 U(9) = 0.581131E+001 U(10) = 0.58376E+001 U(11) = 0.5861E+001 U(12) = 0.588E+001
- U(13) = 0.5E+001
- U(14) = 0.0

The reading functions are adapted to classic floating-point variables, which must be transformed into stochastic variables.

Example:

| Initial C/C++ | Modified statements | | |
|-----------------|---|--|--|
| code | for CADNA | | |
| | <pre>#include <cadna.h></cadna.h></pre> | | |
| float x; | <pre>float_st x;</pre> | | |
| | float xaux; | | |
| | <pre>cadna_init(-1);</pre> | | |
| | | | |
| scanf("%f",&x); | scanf("%f",& xaux); | | |
| | x=xaux; | | |

An example proposed by S. Rump

```
Computation of f(10864, 18817) and f(\frac{1}{3}, \frac{2}{3}) with f(x, y) = 9x^4 - y^4 + 2y^2
#include <stdio.h>
```

```
double rump(double x, double y) {
  double a, b, c;
  a = 9.0 * x * x * x * x;
  b = y * y * y * y;
  c = 2.0 * v * v;
  return a-b+c;
}
int main(int argc, char **argv) {
  double x, y;
  x = 10864.0;
  y = 18817.0;
  printf("%f\n", rump(x, y));
  x = 1.0/3.0;
  v = 2.0/3.0:
  printf("%f\n", rump(x, y));
  return 0:
}
```

Results without CADNA:

P(10864,18817) = 2.000000000000 P(1/3,2/3) = 0.802469135802469E+00

```
double rump(double x, double y) {
  double a, b, c;
  a = 9.0*x*x*x*x;
  b = y*y*y*y;
  c = 2.0*y*y;
  return a-b+c;
}
int main(int argc, char **argv) {
```

```
double x, y;
x = 10864.0;
y = 18817.0;
printf("%f\n", rump(x, y) );"
x = 1.0/3.0;
y = 2.0/3.0;
printf("%f\n", rump(x, y) );"
```

```
return 0;
```

}

#include <stdio.h>

```
#include <stdio.h>
#include <cadna.h>
double rump(double x, double y) {
 double a, b, c;
 a = 9.0 \times x \times x \times x;
 b = y * y * y * y;
 c = 2.0 * y * y;
  return a-b+c;
int main(int argc, char **argv) {
  double x, y;
 x = 10864.0;
  y = 18817.0;
 printf("%f\n", rump(x, y));"
 x = 1.0/3.0;
  y = 2.0/3.0;
 printf("%f\n", rump(x, y));"
```

```
return 0;
```

}

```
#include <stdio.h>
#include <cadna.h>
double rump(double x, double y) {
 double a, b, c;
 a = 9.0 \times x \times x \times x;
 b = y * y * y * y;
 c = 2.0 * v * v;
  return a-b+c;
int main(int argc, char **argv) {
  cadna_init(-1);
  double x, y;
 x = 10864.0;
  y = 18817.0;
 printf("%f\n", rump(x, y));"
 x = 1.0/3.0;
  y = 2.0/3.0;
 printf("%f\n", rump(x, y));"
```

```
return 0;
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}

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 x = 1.0/3.0;
  y = 2.0/3.0;
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  y = 2.0/3.0;
  printf("%f\n", rump(x, y));"
  cadna_end();
  return 0;
}
```

```
#include <stdio.h>
#include <cadna.h>
double_st rump(double_st x, double_st y) {
  double_st a, b, c;
 a = 9.0 \times x \times x \times x;
 b = y * y * y * y;
 c = 2.0 * y * y;
  return a-b+c;
int main(int argc, char **argv) {
  cadna_init(-1);
  double_st x, y;
 x = 10864.0;
  y = 18817.0;
 printf("%f\n", rump(x, y));"
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  c = 2.0 * y * y;
  return a-b+c;
int main(int argc, char **argv) {
  cadna_init(-1);
  double_st x, y;
  x = 10864.0;
  y = 18817.0;
  printf("%s\n", strp(rump(x, y)));"
  x = 1.0/3.0;
  y = 2.0/3.0;
  printf("%s\n", strp(rump(x, y)));"
  cadna_end();
  return 0;
```

CADNA software Self-validation detection: ON Mathematical instabilities detection: ON Branching instabilities detection: ON Intrinsic instabilities detection: ON Cancellation instabilities detection: ON

P(10864,18817) = @.0 P(1/3,2/3) = 0.802469135802469E+000

There are 2 numerical instabilities 2 LOSS(ES) OF ACCURACY DUE TO CANCELLATION(S) The run without CADNA:

$$\begin{array}{l} 9^*x^*x^*x \rightarrow \\ y^*y^*y^*y \rightarrow \\ 9^*x^*x^*x^*x - y^*y^*y^*y \rightarrow \\ 2^*y^*y \rightarrow \\ 9^*x^*x^*x^*x - y^*y^*y^*y + 2y^*y \rightarrow \end{array}$$

1.25372283822342144E+017 1.25372284530501120E+017 -708158976.0000000 708158978.0000000 2.00000000000000000

The run with CADNA:

$$\begin{array}{l} 9^*x^*x^*x \rightarrow \\ y^*y^*y^*y \rightarrow \\ 9^*x^*x^*x^*x - y^*y^*y^*y \rightarrow \\ 2^*y^*y \rightarrow \\ 9^*x^*x^*x^*x - y^*y^*y^*y + 2y^*y \rightarrow \end{array}$$

0.125372283822342E+018 0.125372284530501E+018 -0.7081589E+009 0.708158977999999E+009 @.0

the data_st function

takes into account errors on data by perturbing the samples of a stochastic variable.

- data_st(X): perturbation of the last bit of the mantissa.
- data_st(X, ERX, 0): relative error

$$X_i = X_i * (1 + ERX * ALEA)$$

• data_st(X, ERX, 1): absolute error

$$X_i = X_i + (ERX * ALEA)$$

Example :

float_st b; b=-2.1; data st(b,0.1,0);

The 3 samples become:

-2.309487 -1.980967 -2.100000

F. Jézéquel (LIP6)

- In direct methods:
 - estimate the numerical quality of the results
 - control branching statements
- In iterative methods:
 - optimize the number of iterations
 - check if the computed solution is satisfactory
- In approximation methods:
 - optimize the integration step

```
0.3x^2 - 2.1x + 3.675 = 0
```

Without CADNA, in single precision with rounding to the nearest: d = -3.8146972E-06Two complex roots z1 = 0.3499999E+01 + i * 0.9765625E-03 z2 = 0.3499999E+01 + i * -.9765625E-03With CADNA: d = @.0The discriminant is null

The double real root is 0.3500000E+01

Contribution of CADNA in iterative methods

 $U_{n+1}=F(U_n)$

Without / with CADNA

while (fabs(X-Y) > EPSILON)
{
 X = Y;
 Y = F(X);
}

| With CADNA | |
|----------------|---|
| while (X != Y) | { |
| X = Y; | |
| Y = F(X); | |
| } | |

© optimal stopping criterion

Iterative methods: example

$$S_n(x) = \sum_{i=1}^{i=n} \frac{x^i}{i!}$$

Stopping criterion

• IEEE:
$$|S_n - S_{n-1}| < 10^{-15} |S_n|$$

• CADNA:
$$S_n == S_{n-1}$$

| | IEEE | | CADNA | | |
|------|------|-------------------------|-------|---------------------|--|
| X | iter | $S_n(x)$ | iter | $S_n(x)$ | |
| -5. | 37 | 6.737946999084039E-003 | 38 | 0.673794699909E-002 | |
| -10. | 57 | 4.539992962303130E-005 | 58 | 0.45399929E-004 | |
| -15. | 76 | 3.059094197302006E-007 | 77 | 0.306E-006 | |
| -20. | 94 | 5.621884472130416E-009 | 95 | @.0 | |
| -25. | 105 | -7.129780403672074E-007 | 106 | @.0 | |

Approximation of a limit $L = \lim_{h \to 0} L(h)$

Two kind of errors:

- $e_m(h)$: truncation error (*mathematical* error)
- e_c(h): rounding error (computation error)

If *h* decreases, $e_m(h)$ decreases, but $e_c(h)$ increases.

If *h* decreases, *L*(*h*): s exponent mantissa
$$\leftarrow e_c(h)$$

How to estimate the optimal step?

If $e_c(h) < e_m(h)$, decreasing *h* brings reliable information. Computation should stop when $e_c(h) \approx e_m(h)$

Theorem

Let us consider a numerical method which provides an approximation L(h) of order p to an exact value L:

$$L(h) - L = Kh^p + O(h^q)$$
 with $1 \le p < q$, $K \in \mathbb{R}$.

If L_n is the approximation computed with the step $\frac{h_0}{2^n}$, then

$$C_{L_{n},L_{n+1}} = C_{L_{n},L} + \log_{10}\left(\frac{2^{p}}{2^{p}-1}\right) + O\left(2^{n(p-q)}\right).$$

$$\log_{10}\left(\frac{2^{p}}{2^{p}-1}\right) \le \log_{10}\left(\frac{2}{2-1}\right) = \log_{10}\left(2\right) \approx 0.3$$

If the convergence zone is reached, the digits common to two successive iterates are also common to the exact result, up to one.

The technique of "step halving" is applied and iterations are stopped when $L_n - L_{n-1} = @.0$

You are sure that the result L_n is optimal.

Furthermore its significant digits which are not affected by round-off errors are in common with the exact result *L*, up to one.



Approximations are computed using Simpson's method.

```
1 \text{ Tn} = 0.532202672142964 \text{E} + 002 \text{ err} = 0.459035794670113 \text{E} + 002
n =
   2 Tn=-0.233434428466744E+002 err= 0.306601305939595E+002
n =
   3 Tn=-0.235451792663099E+002 err= 0.308618670135950E+002
n =
   4 Tn= 0.106117380632568E+002 err= 0.329505031597175E+001
n =
n =
   5 Tn= 0.742028156692706E+001 err= 0.1035938196419E+000
   6 Tn= 0.732233719854278E+001 err= 0.564945125770E-002
n =
   7 In= 0.731702967403266E+001 err= 0.34192674758E-003
n =
   8 In= 0.731670894914430E+001 err= 0.2120185922E-004
n =
   9 Tn= 0.731668906978969E+001 err= 0.13225046E-005
n =
n=10 In= 0.731668782990089E+001 err= 0.8261581E-007
n=11 Tr = 0.731668775244794E+001 err = 0.516286E-008
n=12 In= 0.73166877476078E+001 err= 0.3227E-009
n=13 Tr = 0.73166877473053E+001 err = 0.202E-010
n=14 In= 0.73166877472864E+001 err= 0.1E-011
n=15 In= 0.73166877472852E+001 err= 0.1E-012
n=16 Tr = 0.73166877472851E+001 err=0.0
```

The exact solution is: 7.316687747285081429939.

Theorem also valid for the trapezoidal method, Gauss-Legendre method,...

Similar theoretical result for Romberg's method \Rightarrow same strategy: in the result obtained, the digits which are not affected by round-off errors are those of the exact result, up to one.

Also theoretical results for combined sequences \Rightarrow dynamical control of infinite integrals, multidimensional integrals

available on cadna.lip6.fr

- CADNAIZER
 - automatically transforms C codes to be used with CADNA
- CADTRACE
 - identifies the instructions responsible for numerical instabilities

Example:

There are 12 numerical instabilities.

10 LOSS(ES) OF ACCURACY DUE TO CANCELLATION(S). 5 in <ex> file "ex.f90" line 58 5 in <ex> file "ex.f90" line 59

1 INSTABILITY IN ABS FUNCTION.

1 in <ex> file "ex.f90" line 37

1 UNSTABLE BRANCHING.

1 in <ex> file "ex.f90" line 37

SAM (Stochastic Arithmetic in Multiprecision) [Graillat & al.'11]

- implements stochastic arithmetic in arbitrary precision (based on MPFR¹) mp_st stochastic type
- operator overloading \Rightarrow few modifications in user C/C++ programs

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- implements stochastic arithmetic in arbitrary precision (based on MPFR¹) mp_st stochastic type
- operator overloading \Rightarrow few modifications in user C/C++ programs

Recent improvement: control of operations mixing different precisions



 \Rightarrow accuracy estimation on FPGA

¹www.mpfr.org

Other numerical validation tools based on result perturbation

- MCAlib [Frechling et al., 2015]
- VerifiCarlo [Denis et al., 2016] based on LLVM
- Verrou [Févotte et al., 2017] based on Valgrind, no source code modification ③
- asynchronous approach: 1 complete run \rightarrow 1 result, no accuracy analysis during the run
- if branches in the user code: several executions → possibly several branches (require more samples than CADNA)
- no support for GPU codes.

Numerical applications
Example: Mandelbrot set computed on GPU

- We map a 2D image on a part of the complex plane
- for each pixel we iterate at most *N* times:

 $z_{n+1} = z_n^2 + c$, with $z_0 = 0$ and $c \in \mathbb{C}$ the pixel center coordinates.

- If $\exists n \text{ s.t. } |z_n| > 2$, the sequence will diverge and *c* is not in the set.
- Otherwise, *c* is in the set.



Mandelbrot set computed on GPU with CADNA



unstable test $|z_n| > 2 \implies$ complete loss of accuracy in z_n

Should these points be in the set ?

F. Jézéquel (LIP6)

For oil exploration, the 3D acoustic wave equation

$$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} - \sum_{b \in x, y, z} \frac{\partial^2}{\partial b^2} u = 0$$

where *u* is the acoustic pressure, *c* is the wave velocity and *t* is the time

is solved using a finite difference scheme

- time: order 2
- space: order p (in our case p = 8).

2 implementations of the finite difference scheme

$$u_{ijk}^{n+1} = 2u_{ijk}^{n} - u_{ijk}^{n-1} + \frac{c^{2}\Delta t^{2}}{\Delta h^{2}} \sum_{l=-p/2}^{p/2} a_{l} \left(u_{i+ljk}^{n} + u_{ij+lk}^{n} + u_{ijk+l}^{n} \right) + c^{2}\Delta t^{2} f_{ijk}^{n}$$

$$u_{ijk}^{n+1} = 2u_{ijk}^n - u_{ijk}^{n-1} + \frac{c^2 \Delta t^2}{\Delta h^2} \left(\sum_{l=-p/2}^{p/2} a_l u_{i+ljk}^n + \sum_{l=-p/2}^{p/2} a_l u_{ij+lk}^n + \sum_{l=-p/2}^{p/2} a_l u_{ijk+l}^n \right) + c^2 \Delta t^2 f_{ijk}^n$$

where u_{ijk}^n (resp. f_{ik}^n) is the wave (resp. source) field in (i, j, k) coordinates and n^{th} time step and $a_{i \in -p/2, p/2}$ are the finite difference coefficients



1

2

Results depend on :

- the implementation of the finite difference scheme
- the compiler / architecture (various CPUs and GPUs used)

In *binary32*, for $64 \times 64 \times 64$ space steps and 1000 time iterations:

- any two results at the same space coordinates have 0 to 7 common digits
- the average number of common digits is about 4.

Results computed at 3 different points

| scheme | point in the space domain | | | | |
|-----------------------------|---------------------------|---------------------|---------------------|--|--|
| | $p_1 = (0, 19, 62)$ | $p_2 = (50, 12, 2)$ | $p_3 = (20, 1, 46)$ | | |
| AMD Opteron CPU with gcc | | | | | |
| 1 | -1.110479E+0 | 5.454238E+1 | 6.141038E+2 | | |
| 2 | -1.110426E+0 | 5.454199E+1 | 6.141035E+2 | | |
| NVIDIA C2050 GPU with CUDA | | | | | |
| 1 | -1.110204E+0 | 5.454224E+1 | 6.141046E+2 | | |
| 2 | -1.10 9869E+0 | 5.454244E+1 | 6.141047E+2 | | |
| NVIDIA K20c GPU with OpenCL | | | | | |
| 1 | -1.109953E+0 | 5.454218E+1 | 6.141044E+2 | | |
| 2 | -1.11 1517E+0 | 5.454185E+1 | 6.141024E+2 | | |
| AMD Radeon GPU with OpenCL | | | | | |
| 1 | -1.109940E+0 | 5.454317E+1 | 6.141038E+2 | | |
| 2 | -1.11 0111E+0 | 5.454170E+1 | 6.141044E+2 | | |
| AMD Trinity APU with OpenCL | | | | | |
| 1 | -1.110023E+0 | 5.454169E+1 | 6.141062E+2 | | |
| 2 | -1.110113E+0 | 5.454261E+1 | 6.141049E+2 | | |

Results computed at 3 different points

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| 2 | -1.11 0111E+0 | 5.454170E+1 | 6.141044E+2 | | |
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| 1 | -1.110023E+0 | 5.454169E+1 | 6.141062E+2 | | |
| 2 | -1.11 0113E+0 | 5.454261E+1 | 6.141049E+2 | | |

How to estimate the impact of rounding errors?

The acoustic wave propagation code examined with CADNA

The code is run on:

- an AMD Opteron 6168 CPU with gcc
- an NVIDIA C2050 GPU with CUDA.

With both implementations of the finite difference scheme, the number of exact digits varies from 0 to 7 (single precision).

Its mean value is:

- 4.06 with both schemes on CPU
- 3.43 with scheme 1 and 3.49 with scheme 2 on GPU.

 \Rightarrow consistent with our previous observations

Instabilities detected: > 270 000 cancellations

The acoustic wave propagation code examined with CADNA

Results computed at 3 different points using scheme 1:

| | Point in the space domain | | |
|-----------|---------------------------|---------------------|-------------------------------------|
| | $p_1 = (0, 19, 62)$ | $p_2 = (50, 12, 2)$ | <i>p</i> ₃ = (20, 1, 46) |
| IEEE CPU | -1.110479E+0 | 5.454238E+1 | 6.141038E+2 |
| IEEE GPU | -1.110204E+0 | 5.454224E+1 | 6.141046E+2 |
| CADNA CPU | -1.1E+0 | 5.454E+1 | 6.14104E+2 |
| CADNA GPU | -1.11E+0 | 5.45E+1 | 6.1410E+2 |
| Reference | -1.108603879E+0 | 5.454034021E+1 | 6.141041156E+2 |

Despite differences in the estimated accuracy, the same trend can be observed on CPU and on GPU.

- Highest round-off errors impact negligible results.
- Highest results impacted by low round-off errors.

Accuracy distribution on CPU





Numerical validation of a shallow-water (SW) simulation on GPU

 Numerical model (combination of finite difference stencils) simulating the evolution of water height and velocities in a 2D oceanic basin



- Focusing on an eddy evolution:
 - 20 time steps (12 hours of simulated time) on a 1024 × 1024 grid
 - CUDA GPU deployment
 - in double precision



SW eddy simulation with CADNA-GPU

At the end of the simulation:



Square of water velocity in $m^2.s^{-2}$



Number of exact significant digits estimated by

CADNA-GPU

- at eddy center: great accuracy loss equilibrium between several forces (pressure, Coriolis) ⇒ possible cancellations
- point at the very center: 9 exact significant digits lost
 ⇒ no correct digits in SP
- fortunately, velocity values close to zero at eddy center
 - \rightarrow negligible impact on the output
 - \rightarrow satisfactory overall accuracy

Accuracy analysis... and then?

If the results accuracy is not satisfactory...

• higher precision: single → double → quad → arbitrary precision ...and numerical validation!

compensated algorithms

[Kahan'87], [Priest'92], [Ogita & al.'05], [Graillat & al.'09]

- for sum, dot product, polynomial evaluation,...
- results \approx as accurate as with twice the working precision

accurate and reproducible BLAS

- ExBLAS [Collange & al.'15]
- RARE-BLAS [Chohra & al.'16]
- Repro-BLAS [Ahrens & al.'16]
- OzBLAS [Mukunoki & al.'19]

symbolic computation

Can we use reduced or mixed precision to improve performance and energy efficiency?

 mixed precision linear algebra algorithms algorithms designed for mixed precision associated to an error threshold

precision autotuning

- Precimonious [Rubio-Gonzàlez & al.'13]
 - source modification with LLVM
- CRAFT [Lam & al.'13]
 - binary modifications on the operations
- ADAPT [Menon & al.'18]
 - based on algorithmic differentiation
- CRAFT & ADAPT now combined in FloatSmith [Lam & al.'19]

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They rely on comparisons with the highest precision result

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They rely on comparisons with the highest precision result

[Rump'88] $P = 333.75y^6 + x^2(11x^2y^2 - y^6 - 121y^4 - 2) + 5.5y^8 + x/(2y)$ with x = 77617 and v = 33096float. P = 2 571784e+29

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- float: P = 2.571784e+29
- double: P = 1.17260394005318

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- float: P = 2.571784e+29
- double: *P* =1.17260394005318
- quad: P = 1.17260394005317863185883490452018

- Precimonious [Rubio-Gonzàlez & al.'13]
 - source modification with LLVM
- CRAFT [Lam & al.'13]
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[Rump'88] $P = 333.75y^6 + x^2(11x^2y^2 - y^6 - 121y^4 - 2) + 5.5y^8 + x/(2y)$ with x = 77617 and y = 33096

- float: P = 2.571784e+29
- double: *P* =1.17260394005318
- quad: P = 1.17260394005317863185883490452018
- exact: $P \approx -0.827396059946821368141165095479816292$

PROMISE (PRecision OptiMISE) [Graillat & al.'19]

promise.lip6.fr

PROMISE

- provides a mixed precision code (half, single, double, quad) taking into account a required accuracy
- uses CADNA to validate a type configuration
- uses the Delta Debug algorithm [Zeller'09] to search for a valid type configuration with a mean complexity of $O(n \log(n))$ for *n* variables.











Searching for a valid type configuration

PROMISE with 2 types (ex: double & single precision)

From a code in double, the Delta Debug (DD) algorithm finds which variables can be relaxed to single precision.

Searching for a valid type configuration

PROMISE with 2 types (ex: double & single precision)

From a code in double, the Delta Debug (DD) algorithm finds which variables can be relaxed to single precision.

PROMISE with 3 types (ex: double, single & half precision)

The Delta Debug algorithm is applied twice.

Precision auto-tuning using PROMISE

MICADO: simulation of nuclear cores (EDF)

- neutron transport iterative solver
- 11,000 C++ code lines

| # Digits | # double - # float | Speed up | memory gain |
|----------|--------------------------|-------------|----------------|
| 10 | 19-32 | 1.01 | 1.00 |
| 8 | 18-33 | 1.01 | 1.01 |
| 6 | 13-38 | 1.20 | 1.44 |
| 5 4 | 0-51 | 1.32 | 1.62 |

- Speedup, memory gain: w.r.t. double precision
- Speed-up up to 1.32 and memory gain 1.62
- Mixed precision approach successful: speed-up 1.20 and memory gain 1.44

Neural Network Precision Tuning

Q. Ferro, S. Graillat, T. Hilaire, F. Jézéquel, B. Lewandowski, Neural Network Precision Tuning Using Stochastic Arithmetic, 15th International Workshop on Numerical Software Verification, August 2022. http://hal.archives-ouvertes.fr/hal-03682645 Computing system defined by several neurons distributed on different layers



$$x^{(k+1)} = g^{(k+1)} (W^{(k+1)} x^{(k)} + b^{(k+1)})$$

with W the weight matrix, b the bias vector and g the activation function

- Sine NN: approximation of sine function
- MNIST NN: classification of handwritten digits (MNIST Database)
- CIFAR NN: classification of pictures among 10 classes (dogs, cats, deer, car, boat...) (CIFAR10 Database)
- Inverted Pendulum: computation of a Lyapunov function [Chang et al., 2020]









- Neural Networks created and trained in Python code with Keras or PyTorch
- Python scripts to pass them into C++ instrumented code



Approximation of sine function:

- Scalar input
- 3 dense layers with tanh activation function:
 - 20 neurons \rightarrow 21 types to set
 - 6 neurons \rightarrow 7 types to set
 - 1 neuron \rightarrow 2 types to set
- Scalar output
- \Rightarrow 30 types to set in total



Sine NN w/ input=0.5


Sine NN w/ input=0.5



Classification of handwritten digits:

- Input: vector of size 784 (flatten image)
- 2 dense layers:
 - 64 neurons and ReLU activation function
 → 65 types to set
 - 10 neurons and softmax activation function → 11 types to set
- output vector of size 10: probability distribution for the 10 different classes

wikipedia.org

 \Rightarrow 76 types to set in total

MNIST NN w/ input = test_data[61]



MNIST NN w/ input = test_data[61]



Classification of pictures in 10 classes:

- Input: tensor of shape 32x32x3
- 5 layers:
 - Convolutional layer with 32 neurons and ReLU activation function → 33 types to set
 - Max-pooling layer of size $(2x2) \rightarrow 1$ type to set
 - Convolutional layer with 64 neurons and ReLU activation function → 65 types to set
 - Flatten layer \rightarrow 1 type to set
 - Dense layer of 10 neurons and no activation function → 11 types to set
- output vector of size 10
- \Rightarrow 111 types to set in total

| irplane | the state | | 1 | - | 0 | -* | - 10 | 1 |
|-----------|-----------|----------|------|------|-----|----|------|----------|
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| og | 3. A. | - | | 2 | | 1 | 1 | Ņ |
| og | 2 | 10 | - 71 | ٢ | 100 | 5 | | ŝ |
| orse | - And | <u> </u> | 1 | ICAL | 13 | h | 6 | Ť |
| hip | | cair - | d. | - | Ż | N | 1 | <u>a</u> |
| uck | | 1 | | - | | 2 | - | a. |

cs.toronto.edu



CIFAR NN w/ input=test_data[386]



CIFAR NN w/ input=test_data[386]



Learner to find a Lyapunov function:

- Input: state vector $x \in \mathbb{R}^2$
- 2 dense layers with tanh activation function:
 - 6 neurons \rightarrow 7 types to set
 - 1 neuron → 2 types to set
- output vector of size 10
- \Rightarrow 9 types to set in total





Inverted Pendulum w/ input=(0.5,0.5)



Pendulum NN w/ input=(0.5,0.5)



Stochastic arithmetic can estimate which digits are affected by round-off errors and possibly explain reproducibility failures.

- Relatively low overhead
- Support for wide range of codes (GPU, vectorised, MPI, OpenMP)
- Numerical instabilities sometimes difficult to understand in a large code
- Easily applied to real life applications

CADNA has been successfully used for the numerical validation of academic and industrial simulation codes in various domains such as astrophysics, atomic physics, chemistry, climate science, fluid dynamics, geophysics.