# Numerical validation using stochastic arithmetic

Fabienne Jézéquel

LIP6

https://perso.lip6.fr/Fabienne.Jezequel/AFAE.html

### Overview

- 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

# Representation of real numbers

In a floating-point arithmetic using the radix b,

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

is represented by:

- its sign  $\varepsilon$ , 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.

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

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

### The IEEE 754 standard

- 1st version in 1985, to create a uniform standard for floating-point arithmetic across computers
- revisions in 2008 (FMA,...) and 2019

### Formats using the radix 2:

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

# Single / double precision

### IEEE 754 single precision:

⇒ range: 
$$10^{\pm 38}$$
, accuracy:  $u = 2^{-24} \approx 6 \cdot 10^{-8}$ 

### **IEEE 754 double precision:**

1 2 ... 12 13 ....... 64 
$$| \mathbf{s} | | \mathbf{E} + 2^{10} - 1 | a_1 | a_1 | a_{52}$$

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

Remark:  $a_0 = 1$  (hidden bit)

## Lower precision

### Half precision

- binary16 (fp16):
  - 11 bits for the mantissa, 5 for the exponent  $\Rightarrow$  range:  $10^{\pm 5}$ , accuracy:  $u = 2^{-11} \approx 5 \cdot 10^{-4}$
  - used by NVIDIA GPUs, AMD GPUs, ARM NEON, Fujitsu A64FX ARM, ...

#### bfloat16:

- 8 bits for the mantissa, also 8 for the exponent  $\Rightarrow$  range:  $10^{\pm 38}$ , accuracy:  $u = 2^{-8} \approx 4 \cdot 10^{-3}$
- used by Google TPUs, NVIDIA GPUs, AMD GPUs, ARM NEON, Intel Al/Accelerator chips, ...

also fp8-E4M3, fp8-E5M2, ...

# Rounding mode

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

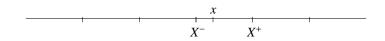
Every real number  $x \notin \mathbb{F}$  is approximated by a number  $X \in \mathbb{F}$ .

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

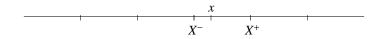
$$X^{-} < x < X^{+} \text{ and } ]X^{-}, X^{+}[ \cap \mathbb{F} = \emptyset$$



How to represent x?

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 x.

**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.

# A significant example - I

#### Let's solve

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

### 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

## A significant example - II

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

• Rounding to +∞ d = 3.81470E-06

There are two different real roots.

x1 = -.3500977E+01x2 = -.3499024E+01

Rounding 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:  $X \cap Y = Y \cap X$
- no associativity:  $(X \cap Y) \cap Z \neq X \cap (Y \cap Z)$
- 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

⇒ it leads to a global inconsistent behaviour.

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

$$X = Y \implies x = y \text{ and } x = y \implies X = Y.$$

$$X \ge Y \implies x \ge y$$
 and  $x \ge y \implies X \ge Y$ .

### 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

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

- p is the number of bits including the hidden bit
- $g_i(d)$  are coefficients depending on data and on the algorithm
- $\alpha_i$  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  $\alpha_i$ .

# A theorem on numerical accuracy

The relative error on R is

$$\left|\frac{R-r}{r}\right| = 2^{-C_R}$$

 $\Rightarrow$  the number of significant bits in common between R and r is

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

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.

# Round-off error analysis

#### 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

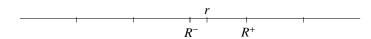
The CESTAC method (Contrôle et Estimation Stochastique des Arrondis de Calculs) was proposed by M. La Porte and J. Vignes in 1974.

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.

## The random rounding mode

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

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

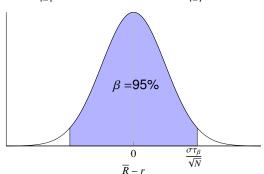
We use the classical Student test which provides a confidence interval of the expectation of a Gaussian distribution from a sample.

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

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

with

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



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

With a probability  $\beta$ ,

$$\left|\overline{R} - r\right| \le \frac{\tau_\beta\,\sigma}{\sqrt{N}}$$

so the number of exact significant digits of  $\overline{R}$ 

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

With a probability  $\beta$ , 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

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

where

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

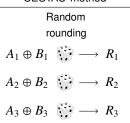
 $\tau_{\beta}$  is the value of Student's distribution for N-1 degrees of freedom and a probability level  $\beta$ .

Classic arithmetic

 $A \oplus B \longrightarrow R$ 

R = 3.14237654356891

#### CESTAC method



 $R_1 = 3.141354786390989$ 

 $R_2 = 3.143689456834534$ 

 $R_3 = 3.142579087356598$ 

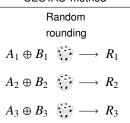
• each operation executed N = 3 times with a random rounding mode

### Classic arithmetic

 $A\oplus B \longrightarrow R$ 

R = 3.14237654356891

#### CESTAC method



 $R_1 = 3.141354786390989$ 

 $R_2 = 3.143689456834534$ 

 $R_3 = 3.142579087356598$ 

- $\bullet$  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%

### On the number of runs

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:

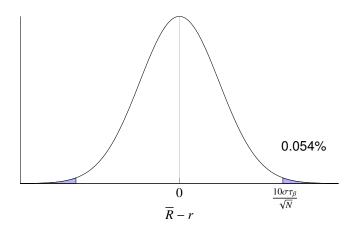
$$P\left(\log_{10}\left(\frac{\sqrt{N}\left|\overline{R}\right|}{\sigma\tau_{\beta}}\right) \ge \log_{10}\left|\frac{\overline{R}}{\overline{R}-r}\right| + 1\right)$$

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

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

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

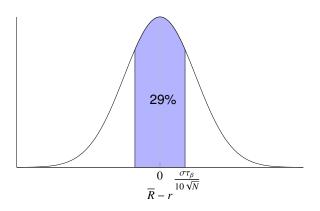
With  $\beta=0.95$  and N=3, the probability of overestimating the number of correct digits of at least 1 is 0.054%



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

$$\begin{split} P\bigg(\log_{10}\bigg(\frac{\sqrt{N}\left|\overline{R}\right|}{\sigma\tau_{\beta}}\bigg) &\leq \log_{10}\bigg|\frac{\overline{R}}{\overline{R}-r}\bigg|-1\bigg) \\ &= P\bigg(\frac{\sqrt{N}\left|\overline{R}\right|}{\sigma\tau_{\beta}} \leq \bigg|\frac{\overline{R}}{10(\overline{R}-r)}\bigg|\bigg) \\ &= P\bigg(\bigg|\frac{\overline{R}}{\overline{R}-r}\bigg| \geq \frac{10\sqrt{N}\left|\overline{R}\right|}{\sigma\tau_{\beta}}\bigg) \\ &= P\bigg(\bigg|\overline{R}-r\bigg| \leq \frac{\sigma\tau_{\beta}}{10\sqrt{N}}\bigg) \end{split}$$

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.

### Self-validation of the CESTAC method

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);
}
```

```
\varepsilon too low \Longrightarrow risk of infinite loop \varepsilon too high \Longrightarrow too early termination.
```

# 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);
}
```

- $\varepsilon$  too low  $\Longrightarrow$  risk of infinite loop
- $\varepsilon$  too high  $\Longrightarrow$  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.

# The concept of computational zero

[Vignes'86]

### Definition

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

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

 $\it R$  is a computed result which, possibly because of round-off errors, cannot be distinguished from  $\it 0$ .

### The stochastic definitions

### Definition

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

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

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

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

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

X is stochastically greater than or equal to Y, noted X s≥ Y, iff

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

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

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

## A few properties

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

# The CADNA library - I



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

## The CADNA library - II

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

## How to implement CADNA

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.

# Declaration 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 CADNA functions to be found by the compiler.

# Initialization of the CADNA library (1)

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.

## Initialization of the CADNA library (2)

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.

## **Termination**

The call to the cadna\_end function should be the last statement.

The cadna\_end function provides a numerical stability report.

# Changes in the type of variables

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

```
\begin{array}{ccc} \text{half} & \Rightarrow & \text{half\_st} \\ \text{float} & \Rightarrow & \text{float\_st} \\ \text{double} & \Rightarrow & \text{double\_st} \end{array}
```

### Example:

```
float_st a,b,c;
double_st e,f,g;
float_st d[6];
```

# Changes in printing statements

Before printing each stochastic variable, it must be transformed into a string by the strp function. This function returns a char \*, therefore formats in print functions should be modified.

Initial C/C++ code	Modified statements for CADNA		
float x;	<pre>#include <cadna.h> float_st x; cadna_init(-1);</cadna.h></pre>		
 printf("%f8.3\n", x);	printf("%s\n", strp(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
```

# Changes in reading statements

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

## Example:

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

# 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:
```

## An example proposed by S. Rump (2)

#### Results without CADNA:

```
#include <stdio.h>
double rump(double x, double y) {
 double a, b, c;
 a = 9.0 \times x \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 \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 \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;
```

```
#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 \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 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));"
  cadna_end();
  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 \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));"
  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 \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));"
  x = 1.0/3.0;
  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 \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_st 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));"
  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 \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("%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;
```

## The run with CADNA

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

There are 2 numerical instabilities 2 LOSS(ES) OF ACCURACY DUE TO CANCELLATION(S)

## Explanation

#### The run without CADNA:

```
9*x*x*x \to y*y*y*y \to 9*x*x*x*x - y*y*y*y \to 2*y*y \to 9*x*x*x*x - y*y*y*y \to 2*y*y \to 9*x*x*x*x - y*y*y*y + 2y*y \to 3*x*x*x*x - y*y*y*y + 2y*y \( \)
```

1.25372283822342144E+017 1.25372284530501120E+017 -708158976.00000000 708158978.000000000 2.00000000000000000

#### The run with CADNA:

$$9*x*x*x*x \rightarrow y*y*y*y \rightarrow 9*x*x*x*x - y*y*y*y \rightarrow 2*y*y \rightarrow 9*x*x*x*x - y*y*y*y +2y*y \rightarrow 9*x*x*x*x - y*y*y*y +2y*y  $\rightarrow$$$

## the data st function

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

- X.data\_st(): perturbation of the last bit of the mantissa.
- X.data st(ERX,0): relative error

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

X.data st (ERX, 1): absolute error

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

### Example:

```
float st b;
b=-2.1:
b.data st(0.1,0);
```

## The 3 samples become:

- -2.309487 -1.980967

-2.100000

## Contributions of CADNA

- 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

# In direct methods - Example

Let's solve

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

Without CADNA, in single precision with rounding to the nearest:

d = -3.8146972E-06

Two complex roots

z1 = 0.3499999E+01 + i \* 0.9765625E-03

z2 = 0.3499999E+01 + i \* -.9765625E-03

#### With CADNA:

$$d = @.0$$

The 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	
ſ	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 methods

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.

$$\begin{array}{c|c} e_m(h) \longrightarrow \\ \hline \text{If $h$ decreases, $L(h)$: } \hline \text{s} & \text{exponent} & \text{mantissa} \\ & \longleftarrow e_c(h) \\ \hline \end{array}$$

How to estimate the optimal step?

If  $e_c(h) < e_m(h)$ , decreasing h brings reliable information.

Computation should stop when  $e_c(h) \approx e_m(h)$ 

# Significant digits in common between two numbers

The number of decimal significant digits in common between two real numbers a and b is defined in  $\mathbb{R}$  by

- for  $a \neq b$ ,  $C_{a,b} = \log_{10} \left| \frac{a+b}{2(a-b)} \right|$
- for all  $a \in \mathbb{R}$ ,  $C_{a,a} = +\infty$

Then 
$$|a - b| = \left| \frac{a+b}{2} \right| 10^{-C_{a,b}}$$
.

If  $C_{a,b} = 3$ , the relative difference between a and b is of the order of  $10^{-3}$  (a and b have 3 significant decimal digits in common).

If 
$$a = 2.4599976$$
 and  $b = 2.4600012$ , then  $C_{a,b} \approx 5.8$ .

The difference due to the sequences of "0" or "9" is illusive.

The significant decimal digits of a and b become actually different from the 6th position.

# Dynamical control of approximation methods

### **Theorem**

Let us consider an approximation L(h) of order p to an exact value L:

$$L(h) - L = Kh^p + \mathcal{O}(h^q)$$
 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

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

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

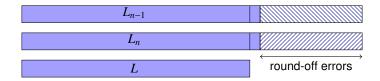
If the convergence zone is reached, the digits common to two successive iterates are also common to the exact result, up to one.

# Approximation methods with the CADNA library

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.



# Approximation methods with the CADNA library

## Ex: approximations computed using Simpson's method

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

The exact solution is: 7.316687747285081429939.

# Dynamical control of approximation methods

Previous theorem also valid for the trapezoidal method, Gauss-Legendre method,...

Similar theoretical result for Romberg's method

⇒ 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

⇒ dynamical control of infinite integrals, multidimensional integrals

## Tools related to CADNA

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

# Libraries for stochastic arithmetic in arbitrary precision

# SAM: Stochastic Arithmetic in Multiprecision

- based on MPFR mpfr.org
- arbitrary mantissa length (exponent length not chosen)
- mantissa length "limited" by RAM
- mp\_st<M> stochastic type
  Ex:
  mp\_st<42>
  mp st<500>

# SAFE: Stochastic Arithmetic with Flexible Exponent

- based on FlexFloat github.com/oprecomp/ flexfloat
- arbitrary mantissa length and arbitrary exponent length
- mantissa length limited by double (or quad) precision
- flexfloat\_st<E,M>
   stochastic type

#### Ex:

flexfloat\_st<8,7> $\Rightarrow$ bf16 flexfloat\_st<5,10> $\Rightarrow$ fp16 flexfloat\_st<5,2> $\Rightarrow$ E5M2

- operator overloading ⇒ few modifications in user C/C++ programs
- control of arithmetic operations mixing several (non-native) formats
- accuracy estimation on FPGA

## Related works

## 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 ©

- $\bullet$  asynchronous approach: 1 complete run  $\to$  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.

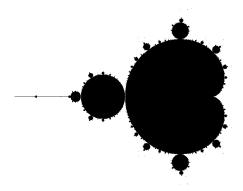
## Numerical applications

### 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:

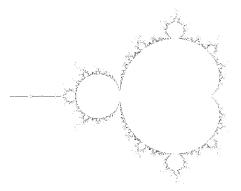
$$z_{n+1} = z_n^2 + c$$
, with  $z_0 = 0$  and  $c \in \mathbb{C}$  the pixel center coordinates.

- 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

#### Pixels with unstable tests:



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

Should these points be in the set?

### Reproducibility failures in a wave propagation code

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

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

is solved using a finite difference scheme

#### 2 implementations of the finite difference scheme

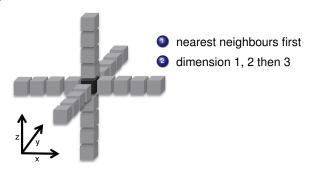
1

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

2

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

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  $a_{l \in -p/2, p/2}$  are the finite difference coefficients



#### Reproducibility problems

#### 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	<b>-1.11</b> 0479E+0	<b>5.454</b> 238E+1	<b>6.1410</b> 38E+2		
2	<b>-1.11</b> 0426E+0	<b>5.454</b> 199E+1	<b>6.1410</b> 35E+2		
NVIDIA C2050 GPU with CUDA					
1	<b>-1.11</b> 0204E+0	<b>5.454</b> 224E+1	<b>6.1410</b> 46E+2		
2	<b>-1.10</b> 9869E+0	<b>5.454</b> 244E+1	<b>6.1410</b> 47E+2		
NVIDIA K20c GPU with OpenCL					
1	<b>-1.10</b> 9953E+0	<b>5.454</b> 218E+1	<b>6.1410</b> 44E+2		
2	<b>-1.11</b> 1517E+0	<b>5.454</b> 185E+1	<b>6.1410</b> 24E+2		
AMD Radeon GPU with OpenCL					
1	<b>-1.10</b> 9940E+0	<b>5.454</b> 317E+1	<b>6.1410</b> 38E+2		
2	<b>-1.11</b> 0111E+0	<b>5.454</b> 170E+1	<b>6.1410</b> 44E+2		
AMD Trinity APU with OpenCL					
1	-1.110023E+0	<b>5.454</b> 169E+1	<b>6.1410</b> 62E+2		
2	<b>-1.11</b> 0113E+0	<b>5.454</b> 261E+1	<b>6.1410</b> 49E+2		

### 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	<b>-1.11</b> 0479E+0	<b>5.454</b> 238E+1	<b>6.1410</b> 38E+2		
2	<b>-1.11</b> 0426E+0	<b>5.454</b> 199E+1	<b>6.1410</b> 35E+2		
NVIDIA C2050 GPU with CUDA					
1	<b>-1.11</b> 0204E+0	<b>5.454</b> 224E+1	<b>6.1410</b> 46E+2		
2	<b>-1.10</b> 9869E+0	<b>5.454</b> 244E+1	<b>6.1410</b> 47E+2		
NVIDIA K20c GPU with OpenCL					
1	<b>-1.10</b> 9953E+0	<b>5.454</b> 218E+1	<b>6.1410</b> 44E+2		
2	<b>-1.11</b> 1517E+0	<b>5.454</b> 185E+1	<b>6.1410</b> 24E+2		
AMD Radeon GPU with OpenCL					
1	<b>-1.10</b> 9940E+0	<b>5.454</b> 317E+1	<b>6.1410</b> 38E+2		
2	<b>-1.11</b> 0111E+0	<b>5.454</b> 170E+1	<b>6.1410</b> 44E+2		
AMD Trinity APU with OpenCL					
1	-1.110023E+0	<b>5.454</b> 169E+1	<b>6.1410</b> 62E+2		
2	<b>-1.11</b> 0113E+0	<b>5.454</b> 261E+1	<b>6.1410</b> 49E+2		

How to estimate the impact of rounding errors?

#### The acoustic wave propagation code 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.
- ⇒ consistent with our previous observations

Instabilities detected: > 270 000 cancellations

# The acoustic wave propagation code examined with CADNA

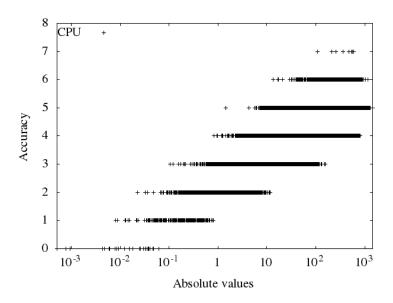
Results computed at 3 different points using scheme 1:

	Point in the space domain		
	$p_1 = (0, 19, 62)$	$p_2 = (50, 12, 2)$	$p_3 = (20, 1, 46)$
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

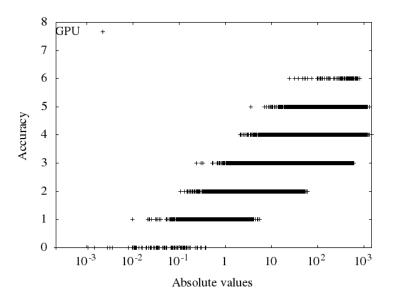
Despite differences in the estimated accuracy, the same trend can be observed on CPU and on GPU.

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

## Accuracy distribution on CPU



## Accuracy distribution on GPU



# 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

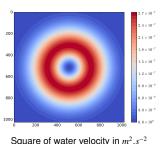


- Focusing on an eddy evolution:
  - 20 time steps (12 hours of simulated time) on a 1024 × 1024 grid
  - CUDA GPU deployment
  - in double precision

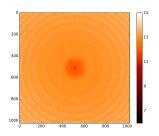


#### SW eddy simulation with CADNA-GPU

#### 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
  - → negligible impact on the output
  - → 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 ≈ 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

- floating-point autotuning tools that intend to deal with large codes:
  - 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]

- floating-point autotuning tools that intend to deal with large codes:
  - Precimonious [Rubio-Gonzàlez & al.'13]
    - source modification with LTVM
  - 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]

They rely on comparisons with the highest precision result



- floating-point autotuning tools that intend to deal with large codes:
  - 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]

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  $y = 33096$  float:  $P = 2.571784e + 29$ 

float:

=2.571784e+29

- floating-point autotuning tools that intend to deal with large codes:
  - 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]

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  $y = 33096$ 

float: P = 2.571784e + 29

double: P = 1.17260394005318

- floating-point autotuning tools that intend to deal with large codes:
  - 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]

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  $y = 33096$ 

float: P = 2.571784e + 29

double: P = 1.17260394005318

quad: P = 1.17260394005317863185883490452018

- floating-point autotuning tools that intend to deal with large codes:
  - 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]

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  $y = 33096$ 

with x = 77617 and y = 33096

float: P = 2.571784e + 29

double: P = 1.17260394005318

quad: P = 1.17260394005317863185883490452018

exact:  $P \approx -0.827396059946821368141165095479816292$ 

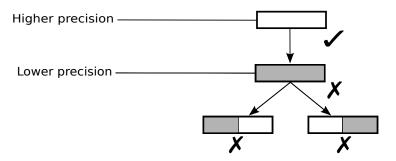
promise.lip6.fr

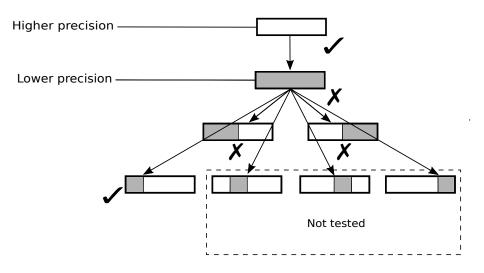
## PROMISE

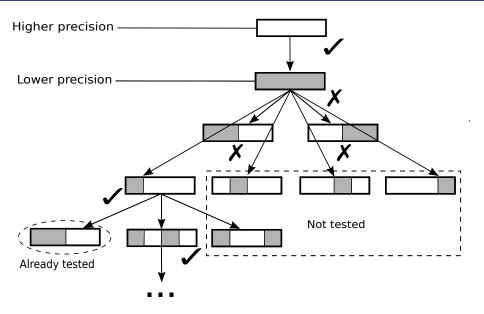
- provides a mixed precision code (half, single, double, quad) taking into account a required accuracy
- uses CADNA to validate a type configuration
- uses the Delta Debug algorithm [Zeller'09] to search for a valid type configuration with a mean complexity of  $O(n \log(n))$  for n variables.



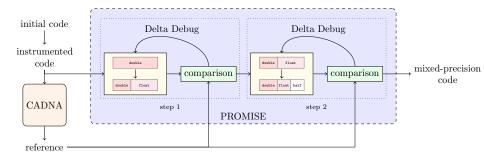








#### PROMISE in double, single and half precision



- step 1: code in double → variables relaxed to single precision
- step 2: single precision variables → variables relaxed to half precision

#### 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

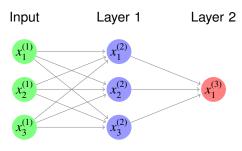
#### Neural Network Precision Tuning

- 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.science/hal-03682645
- Q. Ferro, S. Graillat, T. Hilaire, F. Jézéquel, Performance of precision auto-tuned neural networks, MCSoC 2023 (16th IEEE International Symposium on Embedded Multicore/Manycore Systems-on-Chip) special session POAT (Performance Optimization and Auto-Tuning of Software on Multicore/Manycore Systems), Singapore, December 2023.

https://hal.science/hal-04149501

#### **Neural Network**

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

#### Neural networks studied

- 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]





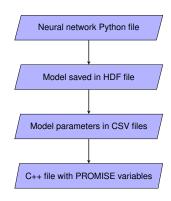




#### Methodology

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

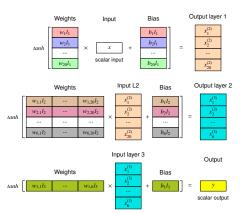
- One type per neuron
- One type per layer
   With input in double precision



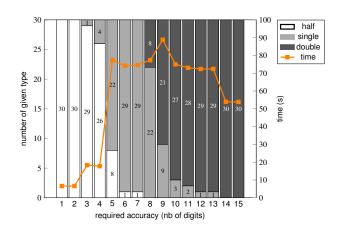
#### Sine NN

#### Approximation of sine function:

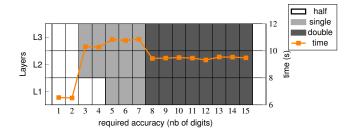
- Scalar input
- 3 dense layers with tanh activation function:
  - 20 neurons → 21 types to set
  - 6 neurons → 7 types to set
  - 1 neuron → 2 types to set
- Scalar output
- ⇒ 30 types to set in total



#### Sine NN w/input=0.5



# Sine NN w/ input=0.5



### MNIST NN

#### Classification of handwritten digits:

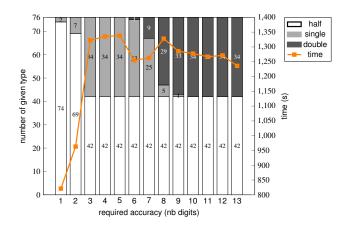
- Input: vector of size 784 (flatten image)
- 2 dense layers:
  - 64 neurons and ReLU activation function  $\rightarrow$  65 types to set
  - 10 neurons and softmax activation function  $\rightarrow$  11 types to set
- output vector of size 10: probability

```
distribution for the 10 different classes
```

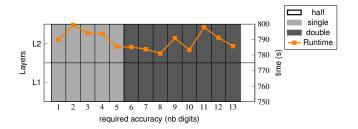
wikipedia.org

 $\Rightarrow$  76 types to set in total

# MNIST NN w/ input = test\_data[61]



### MNIST NN w/ input = test\_data[61]



#### **CIFAR NN**

#### Classification of pictures in 10 classes:

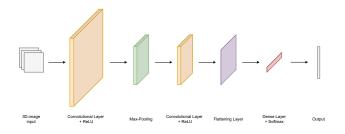
- Input: tensor of shape 32x32x3
- 5 layers:
  - Convolutional layer with 32 neurons and ReLU activation function → 33 types to set
  - Max-pooling layer of size (2x2) → 1 type to set
  - Convolutional layer with 64 neurons and ReLU activation function → 65 types to set
  - Flatten layer → 1 type to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



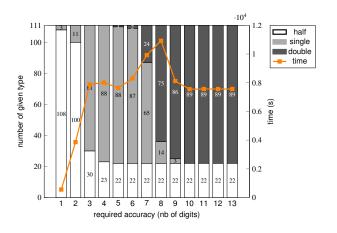
cs.toronto.edu

 $\Rightarrow$  111 types to set in total

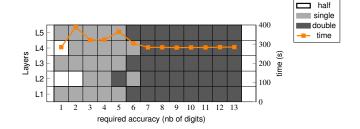
### **CIFAR NN**



# CIFAR NN w/ input=test\_data[386]



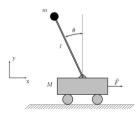
### CIFAR NN w/ input=test\_data[386]



### Pendulum NN

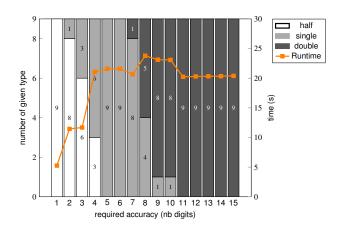
#### Learner to find a Lyapunov function:

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

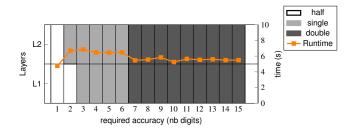


wikipedia.org

### Inverted Pendulum w/ input=(0.5,0.5)



# Pendulum NN w/ input=(0.5,0.5)



### Conclusion

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.

#### References

- J. Vignes, Discrete Stochastic Arithmetic for Validating Results of Numerical Software, Num. Algo., 37, 1–4, p. 377–390, 2004.
- P. Eberhart, J. Brajard, P. Fortin, and F. Jézéquel, High Performance Numerical Validation using Stochastic Arithmetic, Reliable Computing, 21, p. 35–52, 2015.

https://hal.science/hal-01254446

S. Graillat, F. Jézéquel, R. Picot, F. Févotte, and B. Lathuilière, Auto-tuning for floating-point precision with Discrete Stochastic Arithmetic, J. Computational Science, 36, 2019.

https://hal.science/hal-01331917

F. Jézéquel, S. sadat Hoseininasab, T. Hilaire, Numerical validation of half precision simulations, 1st Workshop on Code Quality and Security (CQS 2021), WorldCIST'21, 2021.

https://hal.science/hal-03138494

Q. Ferro, S. Graillat, T. Hilaire, F. Jézéquel, B. Lewandowski, Neural Network Precision Tuning Using Stochastic Arithmetic, 15th Int. Workshop on Numerical Software Verification, 2022.

https://hal.science/hal-03682645

Q. Ferro, S. Graillat, T. Hilaire, F. Jézéquel, Performance of precision auto-tuned neural networks, POAT-2023, within MCSoC-2023.

https://hal.science/hal-04149501

#### Tools related to DSA

- CADNA: http://cadna.lip6.fr
- SAM: https://perso.lip6.fr/Fabienne.Jezequel/SAM
- SAFE: https://perso.lip6.fr/Fabienne.Jezequel/SAFE
- PROMISE: http://promise.lip6.fr