Stochastic arithmetic: presentation and recent developments

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Overview

I - Stochastic arithmetic and the CADNA software

II - Recent developments related to stochastic arithmetic

Overview

Rounding mode

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

Every real number x which is not a floating point number is approximated by a floating point number $X \in \mathbb{F}$.

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

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

such that

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

To choose the rounding mode is to choose 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 plus infinity: x is represented by X^{+}.

Rounding to minus infinity: x is represented by X^{-}.

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

A significant example - I

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

- **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 plus infinity**
  d = 3.81470E-06
  There are two different real roots.
  x1 = -.3500977E+01
  x2 = -.3499024E+01
- **Rounding to minus infinity**
  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
- no associativity
- no distributivity

On a computer, order relationships are the same as in mathematics

$\Longrightarrow$ it leads to a global inconsistent behaviour.

$$X = Y \;\not\Rightarrow\; x = y \quad \text{and} \quad x = y \;\not\Rightarrow\; X = Y.$$
$$X \geq Y \;\not\Rightarrow\; x \geq y \quad \text{and} \quad x \geq y \;\not\Rightarrow\; X \geq Y.$$

Round-off error model

Let $r \in \mathbb{R}$ be the exact result of n elementary arithmetic operations.

On a computer, one obtains the result $R \in \mathbb{F}$ 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 used for the representation including the hidden bit, $g_i(d)$ are coefficients depending only on data and α_i are the round-off errors.

Remark: we have assumed that exponents and signs of intermediate results do not depend on α_i.

A theorem on numerical accuracy

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

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

The last part corresponds to the accuracy which has been 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.

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 that can be obtained by performing this operation on elements from each interval.
  - guaranteed bounds for each computed result
  - the error may be overestimated
  - specific algorithms
- Probabilistic approach
  - uses a random rounding mode
  - estimates the number of exact significant 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 code several times with different round-off error propagations. Then, different results are obtained.

Briefly, the part that is common to all the different results is assumed to be in common also with the mathematical results and the part that is different in the results is affected by the round-off errors.

The random rounding mode

Let r be the result of an arithmetic operation: $R^{-} < r < R^{+}$.

The random rounding mode consists in rounding r to minus infinity or plus infinity with the probability 0.5.

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

By running N times the code with the random arithmetic, one obtains a 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.

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 exact significant decimal digits of $\overline{R}$ with

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

where

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

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

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 exact significant digits given by $C_{\overline{R}}$, we need to multiply the size of the sample 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

With $\beta = 0.95$ and $N = 3$,

- the probability of overestimating the number of exact significant digits of at least 1 is 0.00054
- the probability of underestimating the number of exact significant digits of at least 1 is 0.29.

By choosing a confidence interval at 95%, we prefer to guarantee a minimal number of exact significant digits with 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 a general iterative algorithm be: $U_{n+1} = F(U_n),\ U_0$ being a data.

```
WHILE (ABS(X-Y) $>$ EPSILON) DO
  X = Y
  Y = F(X)
ENDDO
```

ε too low $\Longrightarrow$ a risk of infinite loop
ε too high $\Longrightarrow$ a too early termination.

The optimal choice from the computer point of view:
$X - Y$ **an insignificant value**.

New methods for numerical algorithms may be developed.

The concept of computed zero

J. Vignes, 1986

Definition

Using the CESTAC method, a result R is a computed 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.

The stochastic definitions

Definition

Let X and Y be two computed results using the CESTAC method (N-sample), X is stochastically equal to Y, noted $X \; s\!= \; Y$, if and only if

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

Definition

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

- X is stochastically strictly greater than Y, noted $X \; s\!> \; Y$, if and only if

$$\overline{X} > \overline{Y} \quad \text{and} \quad X \; s\!\neq \; Y$$

- X is stochastically greater than or equal to Y, noted $X \; s\!\geq \; Y$, if and only if

$$\overline{X} \geq \overline{Y} \quad \text{or} \quad X \; s\!= \; Y$$

DSA **Discrete Stochastic Arithmetic** is defined as the joint use of the CESTAC method, the computed zero and the relation definitions.

A few properties

- $x = 0 \implies X = @.0$.
- $X \; s{\neq} \; Y \implies x \neq y$.
- $X \; s{>} \; Y \implies x > y$.
- $x \geq y \implies X \; s{\geq} \; Y$.
- The relation $s{>}$ is transitive.
- The relation $s{=}$ is reflexive, symmetric but not transitive.
- The relation $s{\geq}$ is reflexive, antisymmetric but not transitive.

The CADNA library

The CADNA library implements Discrete Stochastic Arithmetic.

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

More precisely, 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 or C++ programs and also with MPI parallel programs.

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

The stochastic types

CADNA provides two new numerical types, the stochastic types (3 floating point variables `x,y,z` and a hidden variable `acc`):

- `type (single_st)` for stochastic variables in single precision stochastic type associated with real.
- `type (double_st)` for stochastic variables in double precision stochastic type associated with double precision.

All the operators and mathematical functions are overloaded for these types.

The cost of CADNA is about:

- 4 for memory
- 10 for run time.

How to implement CADNA

The use of the CADNA library involves six steps:

- declaration of the CADNA library for the compiler,
- initialization of the CADNA library,
- substitution of the type REAL or DOUBLE PRECISION 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.

An example proposed by S. Rump (1)

Computation of $f(10864, 18817)$ and $f(\frac{1}{3}, \frac{2}{3})$ with $f(x, y) = 9x^4 - y^4 + 2y^2$

```
      program ex1
      implicit double precision (a-h,o-z)
      x = 10864.d0
      y = 18817.d0
      write(*,*)'P(10864,18817) = ', rump(x,y)
      x = 1.d0/3.d0
      y = 2.d0/3.d0
      write(6,100) rump(x,y)
100   format('P(1/3,2/3) = ',e24.15)
      end

      function rump(x,y)
      implicit double precision (a-h,o-z)
      a=9.d0*x*x*x*x
      b=y*y*y*y
      c=2.d0*y*y
      rump = a-b+c
      return
      end
```

An example proposed by S. Rump (2)

The results:

```
P(10864,18817) =    2.00000000000000
P(1/3,2/3) =    0.802469135802469E+00
```

```
program ex1

implicit double precision  (a-h,o-z)

x = 10864.d0
y = 18817.d0
write(*,*)'P(10864,18817) = ', rump(x,y)
x = 1.d0/3.d0
y = 2.d0/3.d0
write(*,*)'P(10864,18817) = ', rump(x,y)

end

function rump(x,y)

implicit double precision  (a-h,o-z)
a = 9.d0*x*x*x*x
b = y*y*y*y
c = 2.d0*y*y
rump = a-b+c
return
end
```

```
program ex1
use cadna
implicit double precision  (a-h,o-z)

x = 10864.d0
y = 18817.d0
write(*,*)'P(10864,18817) = ', rump(x,y)
x = 1.d0/3.d0
y = 2.d0/3.d0
write(*,*)'P(10864,18817) = ', rump(x,y)

end

function rump(x,y)
use cadna
implicit double precision  (a-h,o-z)
a = 9.d0*x*x*x*x
b = y*y*y*y
c = 2.d0*y*y
rump = a-b+c
return
end
```

```
program ex1
use cadna
implicit double precision  (a-h,o-z)
call cadna_init(-1)
x = 10864.d0
y = 18817.d0
write(*,*)'P(10864,18817) = ', rump(x,y)
x = 1.d0/3.d0
y = 2.d0/3.d0
write(*,*)'P(10864,18817) = ', rump(x,y)

end

function rump(x,y)
use cadna
implicit double precision  (a-h,o-z)
a = 9.d0*x*x*x*x
b = y*y*y*y
c = 2.d0*y*y
rump = a-b+c
return
end
```

```
program ex1
use cadna
implicit double precision  (a-h,o-z)
call cadna_init(-1)
x = 10864.d0
y = 18817.d0
write(*,*)'P(10864,18817) = ', rump(x,y)
x = 1.d0/3.d0
y = 2.d0/3.d0
write(*,*)'P(10864,18817) = ', rump(x,y)
call cadna_end()
end

function rump(x,y)
use cadna
implicit double precision  (a-h,o-z)
a = 9.d0*x*x*x*x
b = y*y*y*y
c = 2.d0*y*y
rump = a-b+c
return
end
```

```
program ex1
use cadna
implicit double precision  (a-h,o-z)
call cadna_init(-1)
x = 10864.d0
y = 18817.d0
write(*,*)'P(10864,18817) = ', rump(x,y)
x = 1.d0/3.d0
y = 2.d0/3.d0
write(*,*)'P(10864,18817) = ', rump(x,y)
call cadna_end()
end

function rump(x,y)
use cadna
implicit double precision  (a-h,o-z)
a = 9.d0*x*x*x*x
b = y*y*y*y
c = 2.d0*y*y
rump = a-b+c
return
end
```

```
program ex1
use cadna
implicit type(double_st)  (a-h,o-z)
call cadna_init(-1)
x = 10864.d0
y = 18817.d0
write(*,*)'P(10864,18817) = ', rump(x,y)
x = 1.d0/3.d0
y = 2.d0/3.d0
write(*,*)'P(10864,18817) = ', rump(x,y)
call cadna_end()
end

function rump(x,y)
use cadna
implicit type(double_st)  (a-h,o-z)
a = 9.d0*x*x*x*x
b = y*y*y*y
c = 2.d0*y*y
rump = a-b+c
return
end
```

```
program ex1
use cadna
implicit type(double_st)  (a-h,o-z)
call cadna_init(-1)
x = 10864.d0
y = 18817.d0
write(*,*)'P(10864,18817) = ', rump(x,y)
x = 1.d0/3.d0
y = 2.d0/3.d0
write(*,*)'P(10864,18817) = ', rump(x,y)
call cadna_end()
end

function rump(x,y)
use cadna
implicit type(double_st)  (a-h,o-z)
a = 9.d0*x*x*x*x
b = y*y*y*y
c = 2.d0*y*y
rump = a-b+c
return
end
```

```
program ex1
use cadna
implicit type(double_st)  (a-h,o-z)
call cadna_init(-1)
x = 10864.d0
y = 18817.d0
write(*,*)'P(10864,18817) = ',str(rump(x,y))
x = 1.d0/3.d0
y = 2.d0/3.d0
write(*,*)'P(10864,18817) = ',str(rump(x,y))
call cadna_end()
end

function rump(x,y)
use cadna
implicit type(double_st)  (a-h,o-z)
a = 9.d0*x*x*x*x
b = y*y*y*y
c = 2.d0*y*y
rump = a-b+c
return
end
```

The run with CADNA

```
----------------------------------------------------------------
CADNA software — University P. et M. Curie — LIP6
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
----------------------------------------------------------------
CADNA software — University P. et M. Curie — LIP6
There are 2 numerical instabilities
0 UNSTABLE DIVISION(S)
0 UNSTABLE POWER FUNCTION(S)
0 UNSTABLE MULTIPLICATION(S)
0 UNSTABLE BRANCHING(S)
0 UNSTABLE MATHEMATICAL FUNCTION(S)
0 UNSTABLE INTRINSIC FUNCTION(S)
2 UNSTABLE CANCELLATION(S)
```

Explanation

The run without CADNA:

```
9*x*x*x*x →                    1.2537228382234214E+017
y*y*y*y →                      1.2537228453050112E+017
9*x*x*x*x - y*y*y*y →                   -708158976.00000000
2*y*y →                                  708158978.00000000
9*x*x*x*x - y*y*y*y +2y*y →                       2.0000000000000000
```

The run with CADNA:

```
9*x*x*x*x →                    0.125372283822342E+018
y*y*y*y →                      0.125372284530501E+018
9*x*x*x*x - y*y*y*y →                   -0.7081589E+009
2*y*y →                                  0.708158977999999E+009
9*x*x*x*x - y*y*y*y +2y*y →                   @.0
```

Several versions of the program

	without CADNA	with CADNA

a = 9.d0*x*x*x*x
b = y*y*y*y
c = 2.d0*y*y
rump = a-b+c
	2	@.0

a = 9.d0*x**4
b = y**4
c = 2.d0*y**2
rump = a-b+c
	2	2

rump = 9.d0*x*x*x*x- y*y*y*y + 2.d0*y*y	1	@.0
rump = 9.d0*x**4- y**4 + 2.d0*y**2	1	2

CADNA requires a correct rounding toward $+\infty$ and $-\infty$.

Correct rounding for mathematical functions?

Different mathematical libraries may provide different results: the last bit in the results may differ.

Correct rounding for mathematical functions: an open problem
Extra bits are sometimes required to obtain a correct rounding.

The gnu mathematical library on 64-bit processors:

- provides correct results with rounding to the nearest
- severe bugs may occur with the other rounding modes.

A specific implementation of CADNA exists for 64-bit processors.

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

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

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
```

Iterative methods: which strategy to adopt?

- problems with a solution that cannot be controlled (sequence computation):
  The following stopping criterion should be used

  $$\text{IF}\ \ (x(k).eq.x(k+1))\ \ \text{THEN}$$

- problems with a solution that can be controlled:
  the solution x_s satisfies $\Psi(x_s) = 0$.
  The optimal stopping criterion should be used

  $$\text{IF}\ \ (\Psi(x(k)).eq.0)\ \ \text{THEN}$$

Iterative methods: the solution cannot be controlled

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

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

Iterative methods: the solution can be controlled

The linear system $AX = B$ is solved using Jacobi method.

$$x_i^{(k+1)} = -\frac{1}{a_{ii}} \sum_{j=1, j\neq i}^{n} a_{ij} x_j^{(k)} + \frac{b_i}{a_{ii}}$$

Without CADNA

- Stop when $\max_{i=1}^{n} |x_i^k - x_i^{k-1}| < \varepsilon$
- Compute $R = B - AX^k$.

eps=1.E-3

```
niter =            35
x( 1)= 0.1699924E+01 (exact: 0.1700000E+01), r( 1)= 0.3051758E-03
x( 2)=-0.4746889E+04 (exact:-0.4746890E+04), r( 2)= 0.1953125E-02
x( 3)= 0.5023049E+02 (exact: 0.5023000E+02), r( 3)= 0.1464844E-02
x( 4)=-0.2453197E+03 (exact:-0.2453200E+03), r( 4)=-0.7324219E-03
x( 5)= 0.4778290E+04 (exact: 0.4778290E+04), r( 5)=-0.4882812E-03
x( 6)=-0.7572980E+02 (exact:-0.7573000E+02), r( 6)= 0.9765625E-03
x( 7)= 0.3495430E+04 (exact: 0.3495430E+04), r( 7)= 0.3173828E-02
x( 8)= 0.4350277E+01 (exact: 0.4350000E+01), r( 8)= 0.0000000E+00
x( 9)= 0.4529804E+03 (exact: 0.4529800E+03), r( 9)= 0.9765625E-03
x(10)=-0.2759901E+01 (exact:-0.2760000E+01), r(10)= 0.9765625E-03
x(11)= 0.8239241E+04 (exact: 0.8239240E+04), r(11)= 0.7568359E-02
x(12)= 0.3459919E+01 (exact: 0.3460000E+01), r(12)=-0.4882812E-03
x(13)= 0.1000000E+04 (exact: 0.1000000E+04), r(13)= 0.9765625E-03
x(14)=-0.4999743E+01 (exact:-0.5000000E+01), r(14)= 0.1464844E-02
x(15)= 0.3642400E+04 (exact: 0.3642400E+04), r(15)=-0.1953125E-02
x(16)= 0.7353594E+03 (exact: 0.7353600E+03), r(16)=-0.3662109E-03
x(17)= 0.1700038E+01 (exact: 0.1700000E+01), r(17)= 0.1464844E-02
x(18)=-0.2349171E+04 (exact:-0.2349170E+04), r(18)= 0.1953125E-02
x(19)=-0.8247521E+04 (exact:-0.8247520E+04), r(19)=-0.8728027E-02
x(20)= 0.9843570E+04 (exact: 0.9843570E+04), r(20)= 0.0000000E+00
```

eps=1.E-4

```
niter =          1000
x( 1)= 0.1699924E+01 (exact: 0.1700000E+01), r( 1)= 0.1831055E-03
x( 2)=-0.4746890E+04 (exact:-0.4746890E+04), r( 2)=-0.4882812E-03
x( 3)= 0.5022963E+02 (exact: 0.5023000E+02), r( 3)=-0.9765625E-03
x( 4)=-0.2453193E+03 (exact:-0.2453200E+03), r( 4)= 0.1464844E-02
x( 5)= 0.4778290E+04 (exact: 0.4778290E+04), r( 5)=-0.1464844E-02
x( 6)=-0.7573022E+02 (exact:-0.7573000E+02), r( 6)=-0.1953125E-02
x( 7)= 0.3495430E+04 (exact: 0.3495430E+04), r( 7)= 0.5126953E-02
x( 8)= 0.4350277E+01 (exact: 0.4350000E+01), r( 8)=-0.4882812E-03
x( 9)= 0.4529798E+03 (exact: 0.4529800E+03), r( 9)=-0.9765625E-03
x(10)=-0.2760255E+01 (exact:-0.2760000E+01), r(10)=-0.1953125E-02
x(11)= 0.8239240E+04 (exact: 0.8239240E+04), r(11)= 0.3173828E-02
x(12)= 0.3459731E+01 (exact: 0.3460000E+01), r(12)=-0.1464844E-02
x(13)= 0.1000000E+04 (exact: 0.1000000E+04), r(13)=-0.1953125E-02
x(14)=-0.4999743E+01 (exact:-0.5000000E+01), r(14)= 0.1953125E-02
x(15)= 0.3642400E+04 (exact: 0.3642400E+04), r(15)= 0.0000000E+00
x(16)= 0.7353599E+03 (exact: 0.7353600E+03), r(16)=-0.7324219E-03
x(17)= 0.1699763E+01 (exact: 0.1700000E+01), r(17)=-0.4882812E-03
x(18)=-0.2349171E+04 (exact:-0.2349170E+04), r(18)= 0.0000000E+00
x(19)=-0.8247520E+04 (exact:-0.8247520E+04), r(19)=-0.9155273E-03
x(20)= 0.9843570E+04 (exact: 0.9843570E+04), r(20)=-0.3906250E-02
```

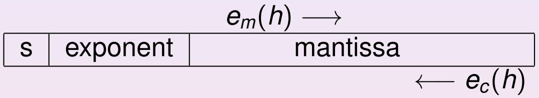
With CADNA

```
 niter =           29
x( 1)= 0.170E+01     (exact: 0.1699999E+01), r( 1)=@.0
x( 2)=-0.4746888E+04 (exact:-0.4746888E+04), r( 2)=@.0
x( 3)= 0.5023E+02    (exact: 0.5022998E+02), r( 3)=@.0
x( 4)=-0.24532E+03   (exact:-0.2453199E+03), r( 4)=@.0
x( 5)= 0.4778287E+04 (exact: 0.4778287E+04), r( 5)=@.0
x( 6)=-0.75729E+02   (exact:-0.7572999E+02), r( 6)=@.0
x( 7)= 0.349543E+04  (exact: 0.3495428E+04), r( 7)=@.0
x( 8)= 0.435E+01     (exact: 0.4349999E+01), r( 8)=@.0
x( 9)= 0.45298E+03   (exact: 0.4529798E+03), r( 9)=@.0
x(10)=-0.276E+01     (exact:-0.2759999E+01), r(10)=@.0
x(11)= 0.823923E+04  (exact: 0.8239236E+04), r(11)=@.0
x(12)= 0.346E+01     (exact: 0.3459999E+01), r(12)=@.0
x(13)= 0.10000E+04   (exact: 0.9999996E+03), r(13)=@.0
x(14)=-0.5001E+01    (exact:-0.4999999E+01), r(14)=@.0
x(15)= 0.364239E+04  (exact: 0.3642398E+04), r(15)=@.0
x(16)= 0.73536E+03   (exact: 0.7353597E+03), r(16)=@.0
x(17)= 0.170E+01     (exact: 0.1699999E+01), r(17)=@.0
x(18)=-0.234917E+04  (exact:-0.2349169E+04), r(18)=@.0
x(19)=-0.8247515E+04 (exact:-0.8247515E+04), r(19)=@.0
x(20)= 0.984356E+04  (exact: 0.9843565E+04), r(20)=@.0
```

Approximation methods

How to estimate the optimal step?

If h decreases, $X(h)$:



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

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

Approximation of integrals

$I = \int_a^b f(x)dx$ is computed using a quadrature method (trapezoidal rule, Simpson's rule, ...)

Let I_n be the approximation computed with step $h = \frac{b-a}{2^n}$.

The computation stops when $I_n - I_{n+1} = @.0$.

```
DO WHILE (integold .NE. integ)
  integold = integ
  h=h/2
  ...
  integ = h * ( ... )
ENDDO
```

Using this strategy, the significant digits of the result which are not affected by round-off errors are in common with I, up to one.

Approximation methods with the CADNA library

Approximation of $\int_{-1}^{1} 20cos(20x)\,((2.7x-3.3)x+1.2)\,dx$ using Simpson's method.

```
n= 1 In= 0.532202672142964E+002 err= 0.459035794670113E+002
n= 2 In=-0.233434428466744E+002 err= 0.306601305939595E+002
n= 3 In=-0.235451792663099E+002 err= 0.308618670135950E+002
n= 4 In= 0.106117380632568E+002 err= 0.329505031597175E+001
n= 5 In= 0.742028156692706E+001 err= 0.103593819641 9E+000
n= 6 In= 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 In= 0.731668906978969E+001 err= 0.13225046E-005
n=10 In= 0.731668782990089E+001 err= 0.8261581E-007
n=11 In= 0.731668775244794E+001 err= 0.516286E-008
n=12 In= 0.73166877476078E+001 err= 0.3227E-009
n=13 In= 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 In= 0.73166877472851E+001 err=@.0
```

The exact solution is: `7.316687747285081429939`.

Overview

I - Stochastic arithmetic and the CADNA software

II - Recent developments related to stochastic arithmetic

- SAM
- CADNA for parallel programs
  - MPI
    - need to define new MPI types for the stochastic types
    - work as for sequential codes
  - OpenMP
    - management of the rounding mode with the threads
    - instability detection
  - GPU
- Parallelization of CADNA

Overview

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The SAM library - I

The SAM library implements in arbitrary precision the features of DSA:

- the stochastic types
- the concept of computational zero
- the stochastic operators.

Arithmetic and relational operators in SAM take into account round-off error propagation.

The particularity of SAM (compared to CADNA) is the arbitrary precision of stochastic variables.

SAM with 24-bit or 53-bit mantissa length is similar to CADNA.

The SAM library - II

- The SAM library is written in C++ and is based on MPFR.
- All operators are overloaded
  $\Mapsto$ for a program in C++ to be used with SAM, only a few modifications are needed.
- Classical variables $\rightarrow$ stochastic variables (of `mp_st` type) consisting of
  - three variables of MPFR type
  - one integer variable to store the accuracy.

Example of SAM code

$$f(x, y) = 333.75y^6 + x^2(11x^2y^2 - y^6 - 121y^4 - 2) + 5.5y^8 + \frac{x}{2y}$$

is computed with $x = 77617$, $y = 33096$.

S. Rump, 1988

```
#include "sam.h"
#include <stdio.h>
int main() {
   sam_init(-1,122);
   mp_st x = 77617; mp_st y = 33096; mp_st res;
   res=333.75*y*y*y*y*y*y+x*x*(11*x*x*y*y-y*y*y*y*y*y
      -121*y*y*y*y-2.0)+5.5*y*y*y*y*y*y*y*y+x/(2*y);
   printf("res=%s\n",strp(res));
   sam_end();
}
```

Output of the SAM code

Using SAM with 122-bit mantissa length, one obtains:

```
SAM software -- University P. et M. Curie -- LIP6
Self-validation detection:  ON
Mathematical instabilities detection:  ON
Branching instabilities detection:  ON
Intrinsic instabilities detection:  ON
Cancellation instabilities detection:  ON
----------------------------
res=-0.827396059946821368141165095479816292
----------------------------
SAM software -- University P. et M. Curie -- LIP6
No instability detected
```

Computation of $f(77617, 33096)$

single precision	1.172603
double precision	1.1726039400531
extended precision	1.172603940053178
Variable precision interval arithmetic	$[-0.827396059946821368141165095479816292005,$ $-0.827396059946821368141165095479816291986]$
SAM, 121 bits	@.0
SAM, 122 bits	$-0.827396059946821368141165095479816292$

Performance test

Run time (in seconds) of SAM and MPFI for the matrix multiplication $M * M$, with $M_{i,j} = i + j + 1$.

Matrix Size: $N = 100$

# bits	24	53	100	500	1000	5000
MPFI	0.292	0.320	0.432	0.504	0.648	2.216
SAM no detection	0.892	0.936	1.076	1.120	1.372	2.616
SAM self-validation	0.896	0.940	1.092	1.160	1.380	2.624
SAM all detections	7.168	8.357	10.461	27.254	69.588	903.528
SAM self-validation/MPFI	3.07	2.94	2.53	2.30	2.13	1.18

The ratio SAM/MPFI is independent of N.

GPU and CADNA

- C++: enough functionalities from CUDA 3.0 for operator and function overloading
- Random functions and the random rounding mode
- Instability detection

The random rounding mode

CPU

```
if (RANDOM) rnd_switch();
res.x=a.x*b.x;   +∞

if (RANDOM) rnd_switch();
res.y=a.y*b.y;   −∞
rnd_switch();
res.z=a.z*b.z;   +∞
```

GPU

```
if (RANDOMGPU())
  res.x=__fmul_ru(a.x,b.x);
else
  res.x=__fmul_rd(a.x,b.x);

if (RANDOMGPU()) {
  res.y=__fmul_rd(a.y,b.y);
  res.z=__fmul_ru(a.z,b.z);
}
else {
  res.y=__fmul_ru(a.y,b.y);
  res.z=__fmul_rd(a.z,b.z);
}
```

2 types: `float_st` for CPU computation and `float_gpu_st` for GPU computation.

Implemented solutions

- No counter for the numerical instabilities
  - need more memory (shared)
  - need a lot of atomic operations
  - instabilities are associated to a result.

CPU +GPU

```
class float_st {
protected:
float x,y,z;
private:
mutable unsigned int accuracy;
unsigned char accuracy;
mutable unsigned char error;
unsigned char pad1, pad2;
}
```

GPU

```
class float_gpu_st {
public:
float x,y,z;
public:
mutable unsigned char accuracy;
mutable unsigned char error;
unsigned char pad1, pad2; }
```

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mutable unsigned int accuracy;
unsigned char accuracy;
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unsigned char pad1, pad2;
}
```

GPU

```
class float_gpu_st {
public:
float x,y,z;
public:
mutable unsigned char accuracy;
mutable unsigned char error;
unsigned char pad1, pad2; }
```

```
#include "cadna.h"
#include "cadna_gpu.cu"

__global__ void matMulKernelNormal(
          float_gpu_st* mat1,
          float_gpu_st* mat2,
          float_gpu_st* matRes,
          int dim) {

  unsigned int x = blockDim.x*blockIdx.x+threadIdx.x;
  unsigned int y = blockDim.y*blockIdx.y+threadIdx.y;

  cadna_init_gpu();

  if (x < dim && y < dim){
    float_gpu_st temp;
    temp=0;
    for(int i=0; i<dim;i++){
      temp = temp + mat1[y * dim + i] * mat2[i * dim + x];
    }
   matRes[y * dim + x] = temp;
  }
}
```

```
...
float_st mat1[DIMMAT][DIMMAT], mat2[DIMMAT][DIMMAT],
         res[DIMMAT][DIMMAT];
...
  cadna_init(-1);
  int size = DIMMAT * DIMMAT * sizeof(float_st);
  cudaMalloc((void **) &d_mat1, size);
  cudaMalloc((void **) &d_mat2, size);
  cudaMalloc((void **) &d_res,  size);
  cudaMemcpy(d_mat1, mat1, size, cudaMemcpyHostToDevice);
  cudaMemcpy(d_mat2, mat2, size, cudaMemcpyHostToDevice);

  dim3 threadsPerBlock(16,16);
  int nbbx = (int)ceil((float)DIMMAT/(float)16);
  int nbby = (int)ceil((float)DIMMAT/(float)16);
  dim3 numBlocks(nbbx , nbby);
  matMulKernelNormal<<< numBlocks , threadsPerBlock>>>
  (d_mat1, d_mat2, d_res, DIMMAT);
  cudaMemcpy(res, d_res,  size, cudaMemcpyDeviceToHost);
  ...
  cadna_end();
```

Scan of the results

```
for(i=0;i<DIMMAT;i++){
    for(j=0;j<DIMMAT;j++)
         printf("%s  ", strp(res[i][j]));
    printf("\n");
}
```

```
mat1=
  0.0000000E+000   0.1000000E+001   0.2000000E+001   0.3000000E+001
  0.4000000E+001   0.5000000E+001   0.6000000E+001   0.6999999E+001
  0.8000000E+001  @.0               0.1000000E+002   0.1099999E+002
  0.1199999E+002   0.1299999E+002   0.1400000E+002   0.1500000E+002


mat2=
  0.1000000E+001   0.1000000E+001   0.1000000E+001   0.1000000E+001
  0.1000000E+001  @.0               0.1000000E+001   0.1000000E+001
  0.1000000E+001   0.1000000E+001   0.1000000E+001   0.1000000E+001
  0.1000000E+001   0.1000000E+001   0.1000000E+001   0.1000000E+001

res=
  0.5999999E+001  @.0                                  0.5999999E+001   0.5999999E+001
  0.2199999E+002  @.0                                  0.2199999E+002   0.2199999E+002
 @.0              @.0              MUL                @.0              @.0
  0.5399999E+002  @.0                                  0.5399999E+002   0.5399999E+002
---------------------------------------------------------------------------------
CADNA GPU software --- University P. et M. Curie --- LIP6
No instability detected on CPU
---------------------------------------------------------------------------------
```

Computation of 2D Slater integrals

2DRMP is a suite of 2D R-matrix propagation programs simulating electron scattering from H-like atoms and ions at intermediate energies. We focus on the NEWRD program which involves the computation of a large number of Slater integrals:

$$I_\lambda = J_{1,\lambda} + J_{2,\lambda}$$

with

$$\begin{aligned}
J_{1,\lambda} &= \int_a^b \int_a^y f_\lambda(x,y)\,dxdy, \\
f_\lambda(x,y) &= \frac{P_{n_1,l_1}(y)P_{n_3,l_3}(y)}{y^{\lambda+1}} x^\lambda P_{n_2,l_2}(x)P_{n_4,l_4}(x), \quad x \in [a,y], \\
J_{2,\lambda} &= \int_a^b \int_y^b \phi_\lambda(x,y)\,dxdy, \\
\phi_\lambda(x,y) &= P_{n_1,l_1}(y)P_{n_3,l_3}(y)y^\lambda \frac{P_{n_2,l_2}(x)P_{n_4,l_4}(x)}{x^{\lambda+1}}, \quad x \in [y,b]
\end{aligned}$$

P_{n_i,l_i}: eigenfunctions of the Schrödinger equation

Performance

- Intel Core 2 Quad Processor Q8200 (4M Cache, 2.33 GHz, 1333 MHz FSB)
- NVIDIA C1060
- NVIDIA C2050 FERMI, CUDA Core 448, Mem 3GB GDDR5

Architecture	time without CADNA	time with CADNA	ratio
CPU	501 sec		
C1060 GPU without texture	26 sec	7 min 22	17
C1060 GPU with texture	21 sec	7 min 15	20.7
C2050 GPU without texture	22 sec	3 min 20	9
C2050 GPU with texture	22 sec	3 min 20	9

All the results are correct with 7 significant digits.

Conclusion

- Efficient method but time and memory consuming
- Can be used on real life applications
- Difficulties to understand the numerical instabilities in large codes
- solution for parallel programs (MPI and GPU)
- difficult to use with the libraries (BLAS, LAPACK ...)

On-going collaborations

- Queen's Univ. of Belfast, UK (atomic physics)
- Institut Pierre Simon Laplace (climate science)
- EDF
- ONERA