Estimation of numerical reproducibility using stochastic arithmetic

Pacôme Eberhart\textsuperscript{1}, Fabienne Jézéquel\textsuperscript{1}, Jean-Luc Lamotte\textsuperscript{1} & Issam Said\textsuperscript{2}

\textsuperscript{1}LIP6, Université Pierre et Marie Curie
\textsuperscript{2}Total & LIP6, Université Pierre et Marie Curie

Retour d’expéRiences sur le Recherche Reproductible (R4)
Orléans, France
3-4 December 2015
Numerical reproducibility failures:

- from one architecture to another
- inside the same architecture.

Different orders in the sequence of instructions
⇒ different round-off errors

differences in results may be difficult to identify: round-off errors or bug?

Stochastic arithmetic can estimate which digits in the results are different from one execution to another because of round-off errors.
Outline

1. Reproducibility failures in a wave propagation code
2. Principles of stochastic arithmetic
3. The CADNA library
4. Porting CADNA for CPU-GPU simulation
5. The wave propagation code examined with stochastic arithmetic
6. Improving CADNA performance and supporting vectorised codes
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

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

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

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

where \( u_{ijk}^n \) (resp. \( f_{ijk}^n \)) 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

- nearest neighbours first
- dimension 1, 2 then 3
Reproducibility problems

- differences from one implementation of the finite difference scheme to another
- differences from one execution to another inside a GPU
  repeatability problem due to differences in the order of thread executions
- differences from one architecture to another

In binary 32, 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

<table>
<thead>
<tr>
<th>scheme</th>
<th>point in the space domain</th>
<th>( p_1 = (0, 19, 62) )</th>
<th>( p_2 = (50, 12, 2) )</th>
<th>( p_3 = (20, 1, 46) )</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>AMD Opteron CPU with gcc</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>-1.110479E+0</td>
<td>5.454238E+1</td>
<td>6.141038E+2</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>-1.110426E+0</td>
<td>5.454199E+1</td>
<td>6.141035E+2</td>
<td></td>
</tr>
<tr>
<td><strong>NVIDIA C2050 GPU with CUDA</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>-1.110204E+0</td>
<td>5.454224E+1</td>
<td>6.141046E+2</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>-1.109869E+0</td>
<td>5.454244E+1</td>
<td>6.141047E+2</td>
<td></td>
</tr>
<tr>
<td><strong>NVIDIA K20c GPU with OpenCL</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>-1.109953E+0</td>
<td>5.454218E+1</td>
<td>6.141044E+2</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>-1.111517E+0</td>
<td>5.454185E+1</td>
<td>6.141024E+2</td>
<td></td>
</tr>
<tr>
<td><strong>AMD Radeon GPU with OpenCL</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>-1.109940E+0</td>
<td>5.454317E+1</td>
<td>6.141038E+2</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>-1.110111E+0</td>
<td>5.454170E+1</td>
<td>6.141044E+2</td>
<td></td>
</tr>
<tr>
<td><strong>AMD Trinity APU with OpenCL</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>-1.110023E+0</td>
<td>5.454169E+1</td>
<td>6.141062E+2</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>-1.110113E+0</td>
<td>5.454261E+1</td>
<td>6.141049E+2</td>
<td></td>
</tr>
</tbody>
</table>
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 $X_{\text{min}}$ (resp. $X_{\text{max}}$) be the smallest (resp. the greatest) floating point number:

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

such that

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

To choose the rounding mode is to choose the algorithm that, according to $x$, gives $X^-$ or $X^+$. 
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

\[ 0.3 \times x^2 + 2.1 \times x + 3.675 = 0 \]

- **Rounding to nearest**
  \[ d = -3.81470E-06 \]
  There are two conjugate complex roots.
  \[ z1 = -.3500000E+01 + i \times 0.9765625E-03 \]
  \[ z2 = -.3500000E+01 + i \times -.9765625E-03 \]

- **Rounding to zero**
  \[ d = 0. \]
  The discriminant is null.
  The double real root is -.3500000E+01
A significant example - II

\[ 0.3 \times x^2 + 2.1 \times x + 3.675 = 0 \]

- **Rounding to plus infinity**
  
  \[ d = 3.81470E-06 \]
  
  There are two different real roots.
  
  \[ x_1 = -.3500977E+01 \]
  
  \[ x_2 = -.3499024E+01 \]

- **Rounding to minus infinity**
  
  \[ d = 0. \]
  
  The discriminant is null.
  
  The double real root is \(-.3500000E+01\)
How to estimate the impact of round-off errors?

The exact result $r$ of an arithmetic operation is approximated by a floating-point number $R^-$ or $R^+$. 

$$
\begin{array}{c}
\hline
& r \\
R^- & & R^+ \\
\hline
\end{array}
$$

The random rounding mode

Approximation of $r$ by $R^-$ or $R^+$ with the probability 1/2

The CESTAC method

The same code is run several times with the random rounding mode. Then different results are obtained.

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

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

\( p \) is the number of bits used for the representation including the hidden bit, \( g_i(d) \) are coefficients depending only on data and \( \alpha_i \) are the round-off errors.

Remark: we have assumed that exponents and signs of intermediate results do not depend on \( \alpha_i \).
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

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

where

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

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

In practice, $N = 3$ and $\beta = 95\%$. 

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 concept of computed zero

J. Vignes, 1986

Definition

Using the CESTAC method, a result $R$ is a computed zero, denoted by $\circ @.0$, if

$$\forall i, R_i = 0 \text{ or } C_R \leq 0.$$ 

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 results computed using the CESTAC method (\( N \)-sample), \( X \) is stochastically equal to \( Y \), noted \( X \ sam Y \), 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
  \[
  \overline{X} \geq \overline{Y} \quad \text{or} \quad X \ s= Y
  \]

Discrete Stochastic Arithmetic (DSA) is defined as the joint use of the CESTAC method, the computed zero and the stochastic relation definitions.
The CADNA library implements Discrete Stochastic Arithmetic.

CADNA allows to **estimate round-off error propagation** in any scientific program written in Fortran or in C++.

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.
The CADNA library implements Discrete Stochastic Arithmetic.

CADNA allows to **estimate round-off error propagation** in any scientific program written in Fortran or in C++.

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 provides new numerical types, the **stochastic types**, which consist of:

- 3 floating point variables
- an integer variable to store the accuracy.

All operators and mathematical functions are redefined for these types.

⇒ **CADNA requires only a few modifications in user programs.**
An example proposed by S. Rump

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

```fortran
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
```

Pacôme Eberhart
Est. of numerical repro. using stochastic arith.
3-4 Dec. 2015 19 / 39
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
derend
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()
dend

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
dend
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) = ', 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
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

defunction 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

---

\[ P(10864,18817) = 0.0 \]
\[ P(1/3,2/3) = 0.802469135802469E+000 \]

---

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 LOSS(ES) OF ACCURACY DUE TO CANCELLATION(S)
**Rounding mode change (until recently):** the *rnd_switch* function
- switches the rounding mode from $+\infty$ to $-\infty$, or from $-\infty$ to $+\infty$.
- is written in assembly language
- changes two bits in the FPU Control Word.
CADNA on CPU

- **Rounding mode change (until recently):** the `rnd_switch` function
  - switches the rounding mode from $+\infty$ to $-\infty$, or from $-\infty$ to $+\infty$.
  - is written in assembly language
  - changes two bits in the FPU Control Word.

- **Instability detection:**
  - dedicated counters are incremented
  - the occurrence of each kind of instability is given at the end of the run.
CADNA for CPU-GPU simulations

**Rounding mode change**
An arithmetic operation on GPU can be performed with a specified rounding mode.

### CPU

```c
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

```c
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
Instability detection

- No counter: would need more memory (shared) and would need a lot of atomic operations
- An unsigned char is associated with each result (each bit is associated with a type of instability).

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

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

- No counter: would need more memory (shared) and would need a lot of atomic operations
- An unsigned char is associated with each result (each bit is associated with a type of instability).

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

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

- No counter: would need more memory (shared) and would need a lot of atomic operations
- An unsigned char is associated with each result (each bit is associated with a type of instability).

```cpp
// 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;
}
```
Example: matrix multiplication

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

__global__ void matMulKernel(
    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;
    }
}
```
Example: matrix multiplication

```c
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);
matMulKernel<<< numBlocks , threadsPerBlock>>>
(d_mat1, d_mat2, d_res, DIMMAT);
cudaMemcpy(res, d_res, size, cudaMemcpyDeviceToHost);
...  
cadna_end();
```
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
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.

⇒ 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:

<table>
<thead>
<tr>
<th>Point in the space domain</th>
<th>$p_1 = (0, 19, 62)$</th>
<th>$p_2 = (50, 12, 2)$</th>
<th>$p_3 = (20, 1, 46)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>IEEE CPU</td>
<td>-1.110479E+0</td>
<td>5.454238E+1</td>
<td>6.141038E+2</td>
</tr>
<tr>
<td>IEEE GPU</td>
<td>-1.110204E+0</td>
<td>5.454224E+1</td>
<td>6.141046E+2</td>
</tr>
<tr>
<td>CADNA CPU</td>
<td>-1.1E+0</td>
<td>5.454E+1</td>
<td>6.14104E+2</td>
</tr>
<tr>
<td>CADNA GPU</td>
<td>-1.11E+0</td>
<td>5.45E+1</td>
<td>6.1410E+2</td>
</tr>
<tr>
<td>Reference</td>
<td>-1.108603879E+0</td>
<td>5.454034021E+1</td>
<td>6.141041156E+2</td>
</tr>
</tbody>
</table>

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 graph on CPU](image-url)

- **Accuracy** on the Y-axis
- **Absolute values** on the X-axis
Accuracy distribution on GPU

Accuracy

Absolute values

GPU

Est. of numerical repro. using stochastic arith.

3-4 Dec. 2015
## Execution times

<table>
<thead>
<tr>
<th>execution</th>
<th>instability detection</th>
<th>CPU execution time (s)</th>
<th>GPU execution time (s)</th>
<th>ratio</th>
<th>ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>IEEE</td>
<td>all instabilities</td>
<td>110.8</td>
<td>0.80</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>CADNA</td>
<td>no instability</td>
<td>4349</td>
<td>5.73</td>
<td>39.3</td>
<td>7.2</td>
</tr>
<tr>
<td></td>
<td>mul., div., branching</td>
<td>1655</td>
<td></td>
<td>14.9</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1663</td>
<td></td>
<td>15.0</td>
<td></td>
</tr>
</tbody>
</table>
Overhead of the CADNA library

There is an overhead in computation time when using the CADNA library.
- A factor of 10 to 40 depending on the program and the level of detection
- Can go up to 2 orders of magnitude for optimised programs
- Mainly due to the change of the FPU rounding mode

Additionally, the lack of support in gcc for directed rounding modes prevents compiler optimisation.
To remove the change of the rounding mode during the computation, we can obtain the values of rounded up operations, using only rounded down operations, thank to the following properties.

- \( a \oplus_{+\infty} b = - (a \oplus_{-\infty} -b) \) (similarly for \( \ominus \))
- \( a \otimes_{+\infty} b = - (a \otimes_{-\infty} -b) \) (similarly for \( \oslash \))

Moreover, this allows for several additional optimisations to be applied.

- Compiler optimisation now possible
- Inlining operators to decrease cost of function calls

Furthermore, to enable support for vectorised codes, we have changed the random generator.
Scalar performance

- **Addition**
  - Execution time (s)
  - IEEE 1.1.9
  - Mask O0: x 53.9
  - Mask O3: x 38.0
  - Inline: x 21.4
  - Dyn: x 10.8
  - Overhead: x 53.9

- **Multiplication**
  - Execution time (s)
  - IEEE 1.1.9
  - Mask O0: x 54.4
  - Mask O3: x 40.1
  - Inline: x 15.1
  - Dyn: x 10.9
  - Overhead: x 54.4

- **Mandelbrot**
  - Execution time (s)
  - IEEE 1.1.9
  - Mask O0: x 114
  - Mask O3: x 78.2
  - Inline: x 35.5
  - Dyn: x 22.7
  - Overhead: x 35.5

- **Stencil**
  - Execution time (s)
  - IEEE 1.1.9
  - Mask O0: x 107
  - Mask O3: x 72.9
  - Inline: x 37.8
  - Dyn: x 22.2
  - Overhead: x 22.2
We use \texttt{ispc} (Intel SPMD Program Compiler) to generate vectorised codes.
  
  - Generates for different instructions sets (AVX, SSE, ...) without using intrinsics
  
  - Can define variables as lane specific or vector global

We test two versions of the vectorised CADNA library.
  
  - \texttt{dyn}, directly adapted from the scalar version
  
  - \texttt{define}, where anomaly detection is defined at compile time
Vectorised performance

Addition

Execution time (s)

IEEE - scal
IEEE - AVX2
dyn - scal
dyn - AVX2
define - scal
define - AVX2

Speedup
x 7.8
x 2.2
x 2.4

Multiplication

Execution time (s)

IEEE - scal
IEEE - AVX2
dyn - scal
dyn - AVX2
define - scal
define - AVX2

Speedup
x 7.7
x 2.4
x 3.6

Mandelbrot

Execution time (s)

IEEE - scal
IEEE - AVX2
dyn - scal
dyn - AVX2
define - scal
define - AVX2

Speedup
x 5.8
x 3.1
x 2.9

Stencil

Execution time (s)

IEEE - scal
IEEE - AVX2
dyn - scal
dyn - AVX2
define - scal
define - AVX2

Speedup
x 3.8
x 2.6
x 2.5
Conclusion

- Measure reliability of numerical applications
- Estimation of the number of exact significant digits
- Relatively low overhead
- Support for wide range of codes (GPU, vectorised, MPI, OpenMP)
- Easily applied to real life applications
- Numerical instabilities sometimes difficult to understand in a big code