Precision auto-tuning and control of accuracy in high performance simulations

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“Optimising Floating-Point Precision” workshop
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Introduction

Floating-point arithmetic: | Sign | Exponent | Mantissa |

Various floating-point formats:

	#bits Mantissa (p)	Exp.	Range	$u = 2^{-p}$
bfloat16 (half)	8	8	$10^{\pm 38}$	$\approx 4 \times 10^{-3}$
fp16 (half)	11	5	$10^{\pm 5}$	$\approx 5 \times 10^{-4}$
fp32 (single)	24	8	$10^{\pm 38}$	$\approx 6 \times 10^{-8}$
fp64 (double)	53	11	$10^{\pm 308}$	$\approx 1 \times 10^{-16}$
fp128 (quad)	113	15	$10^{\pm 4932}$	$\approx 1 \times 10^{-34}$

↘ precision:

- ↘ execution time ☺
- ↘ volume of results exchanged ☺
- ↗ energy efficiency ☺

energy consumption proportional to p^2 [Jouppi et al'20]

energy ratio	
fp64/fp32	≈ 5
fp32/fp16	≈ 5
fp32/bfloat16	≈ 9

- But computed results may be invalid because of rounding errors ☹

Outline

In this talk we aim at answering the following questions.

1. How to control the validity of (mixed precision) floating-point results?
2. How to determine automatically the suitable format for each variable?

Rounding error analysis

Several approaches

- Interval arithmetic
  - guaranteed bounds for each computed result
  - the error may be overestimated
  - specific algorithms
  - ex: INTLAB [Rump'99]
- Static analysis
  - no execution, rigorous analysis, all possible input values taken into account
  - not suited to large programs
  - ex: FLUCTUAT [Goubault & al.'06], FLDLib [Jacquemin & al.'19]
- Probabilistic approach
  - estimates the number of correct digits of any computed result
  - requires no algorithm modification
  - can be used in HPC programs
  - ex: CADNA [Chesneaux'90], SAM [Graillat & al.'11], VERIFICARLO [Denis & al.'16], VERROU [Févotte & al.'17]

Discrete Stochastic Arithmetic (DSA) [Vignes'04]

Classic arithmetic

$A \oplus B \longrightarrow R$

R =3.14237654356891

DSA

Random rounding

$A_1 \oplus B_1 \longrightarrow R_1$

$A_2 \oplus B_2 \longrightarrow R_2$

$A_3 \oplus B_3 \longrightarrow R_3$

R_1 =**3.14**1354786390989
R_2 =**3.14**3689456834534
R_3 =**3.14**2579087356598

- each operation executed 3 times with a random rounding mode

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

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- each operation executed 3 times with a random rounding mode
- number of correct digits in the results estimated using Student's test with the confidence level 95%
- operations executed synchronously
  - ⇒ detection of numerical instabilities
    Ex: `if (A>B)` with `A-B` numerical noise
  - ⇒ optimization of stopping criteria

The CADNA library

cadna.lip6.fr

- implements stochastic arithmetic for C/C++ or Fortran codes
- provides stochastic types (3 floating-point variables and an integer)
- all operators and mathematical functions overloaded
  $\Rightarrow$ few modifications in user programs
- support for MPI, OpenMP, GPU codes
- in one CADNA execution: accuracy of any result, complete list of numerical instabilities

[Chesneaux'90], [Jézéquel & al'08], [Lamotte & al'10], [Eberhart & al'18],...

CADNA performance

CADNA cost

- memory: 4
- run time $\approx$ 10

Efficient rounding mode change

- implicit change of the rounding mode thanks to

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

$\bigcirc_{+\infty}$ (resp. $\bigcirc_{-\infty}$): floating-point operation rounded $\rightarrow +\infty$ (resp. $-\infty$)

$\Rightarrow$ no explicit change of the rounding mode

An example without/with CADNA

Computation of $P(x,y) = 9x^4 - y^4 + 2y^2$ [Rump'83]

```
#include <iostream>
using namespace std;
double rump(double x, double y) {
  return 9.0*x*x*x*x - y*y*y*y + 2.0*y*y;
}
int main() {
  cout.precision(15);
  cout.setf(ios::scientific,ios::floatfield);
  double x, y;
  x = 10864.0;
  y = 18817.0;
  cout<<"P1="<<rump(x, y)<< endl;
  x = 1.0/3.0;
  y = 2.0/3.0;
  cout<<"P2="<<rump(x, y)<< endl;
  return 0;
}
```

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  cout<<"P2="<<rump(x, y)<< endl;
  return 0;
}
```

P1=2.00000000000000e+00

P2=8.02469135802469e–01

```
#include <iostream>

using namespace std;
double   rump(double   x, double   y) {
  return 9.0*x*x*x*x-y*y*y*y+2.0*y*y;
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int main() {
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  return 9.0*x*x*x*x-y*y*y*y+2.0*y*y;
}
int main() {
  cout.precision(15);
  cout.setf(ios::scientific,ios::floatfield);
  cadna_init(-1);
  double   x, y;
  x=10864.0; y=18817.0;
  cout«"P1="«rump(x, y)«endl;
  x=1.0/3.0; y=2.0/3.0;
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  return 0;
}
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  cadna_end();
  return 0;
}
```

```
#include <iostream>
#include <cadna.h>
using namespace std;
double_st rump(double_st x, double_st y) {
  return 9.0*x*x*x*x-y*y*y*y+2.0*y*y;
}
int main() {
  cout.precision(15);
  cout.setf(ios::scientific,ios::floatfield);
  cadna_init(-1);
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  cadna_end();
  return 0;
}
```

Remark: CADNAIZER available on `cadna.lip6.fr`

Results with CADNA

only correct digits are displayed

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

P1= @.0 (no correct digits)
P2= 0.802469135802469E+000

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

Stochastic types in CADNA

`half_st   float_st   double_st`

Half precision in CADNA

control of fp16 computation with

- emulated half precision thanks to the library developed by C. Rau (`http://half.sourceforge.net`)
- native half precision on e.g. GPUs or ARM CPUs ≥v8.2 (successful tests on Fugaku supercomputer)

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>

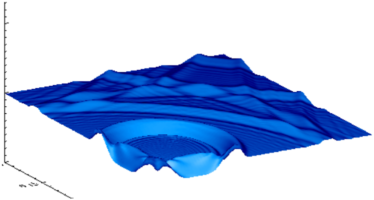
SAFE: Stochastic Arithmetic with Flexible Exponent

- 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>⇒bf16
  flexfloat_st<5,10>⇒fp16
  flexfloat_st<5,2>⇒E5M2

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

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

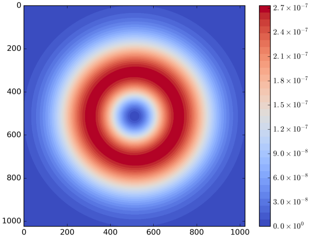
- Simulation of the evolution of water height and velocities in a 2D oceanic basin
- CUDA GPU code in double precision



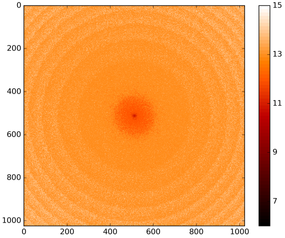
- Focusing on an eddy evolution:
  20 time steps (12 hours of simulated time) on a 1024 × 1024 grid

SW eddy simulation with CADNA-GPU

At the end of the simulation:



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



Number of correct digits estimated by CADNA-GPU

- at eddy center: great accuracy loss due to cancellations
- point at the very center: 9 digits lost
  ⇒ **no correct digits in single precision**
- 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
  ⚠ numerical validation

- **compensated algorithms**
  - for sum, dot product, polynomial evaluation,...
  - results ≈ as accurate as with twice the working precision

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

- **accurate and reproducible BLAS**
  - ExBLAS
    https://github.com/riakymch/exblas
  - Repro-BLAS
    https://bebop.cs.berkeley.edu/reproblas
  - OzBLAS
    https://github.com/mukunoki/ozblas

When the results accuracy is satisfactory...

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

- **mixed precision linear algebra algorithms**
  design of a mixed precision version of specific algorithms
  with an error analysis

  Surveys: [Abdelfattah et al'21, Higham & Mary'22, Kashi et al'24]

- **precision autotuning**
  automatic search for a valid mixed precision types configuration
  whatever the user algorithms

Precision autotuning

Static tools

- FPTaylor/FPTuner [Solovyev & al'15] symbolic Taylor expansions
- DAISY [Darulova & al'18] mixed-precision with rewriting
- TAFFO [Cherubin & al'19] auto-tuning for floating to fixed-point optimization
- POP [Ben Khalifa & al'19] error analysis by constraint generation

not suited to large scale programs ☹

Precision autotuning

Dynamic tools

intend to deal with large codes

- CRAFT [Lam & al'13] binary modifications on the operations
- Precimonious [Rubio-Gonzàlez & al'13] source modification with LLVM
- Blame Analysis [Nguyen & al'15] improves Precimonious
- HiFPTuner [Guo & al'18] based on a hierarchical search algorithm
- ADAPT [Menon & al'18] based on algorithmic differentiation
- FloatSmith [Lam & al'19] combination of CRAFT & ADAPT
- FPLearner [Wang & Rubio-Gonzàlez'24] improves precision tuners using ML
- Tools dedicated to GPUs (that pay attention to casts):
  - AMPT-GA [Kotipalli & al'19]
  - GPUMixer [Laguna & al'19]
  - GRAM [Ho & al'21]

Precision autotuning

Dynamic tools 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

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float: $P =$2.571784e+29

double: $P =$1.17260394005318

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with $x = 77617$ and $y = 33096$

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

Precision autotuning

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with $x = 77617$ and $y = 33096$

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

PROMISE (PRecision OptiMISE) [Graillat & al'19], [F.J. & al'21], ...

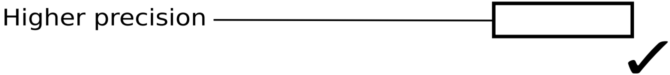
promise.lip6.fr

PROMISE

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

Searching for a valid configuration with 2 types

Method based on the Delta Debug algorithm [Zeller'09]



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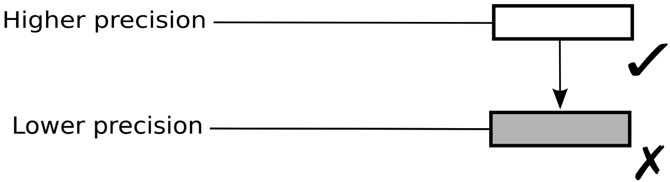

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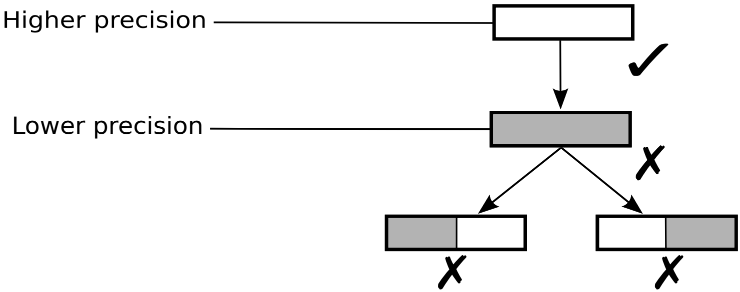

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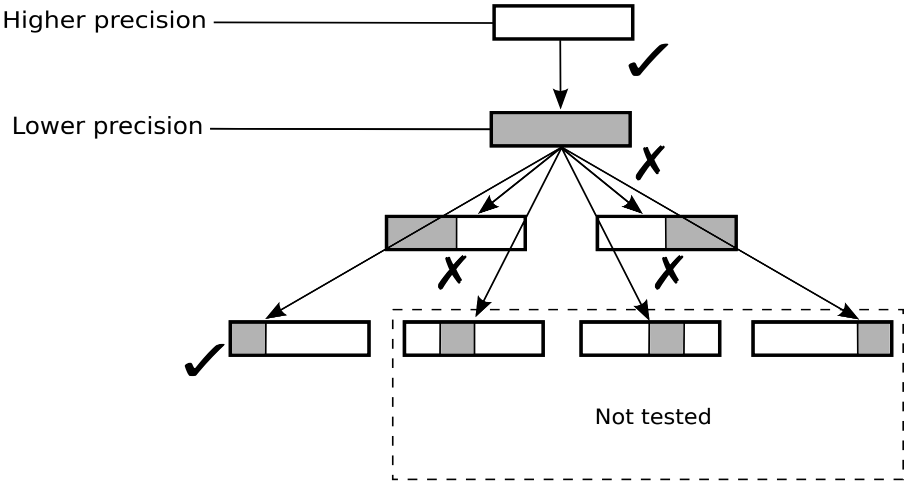

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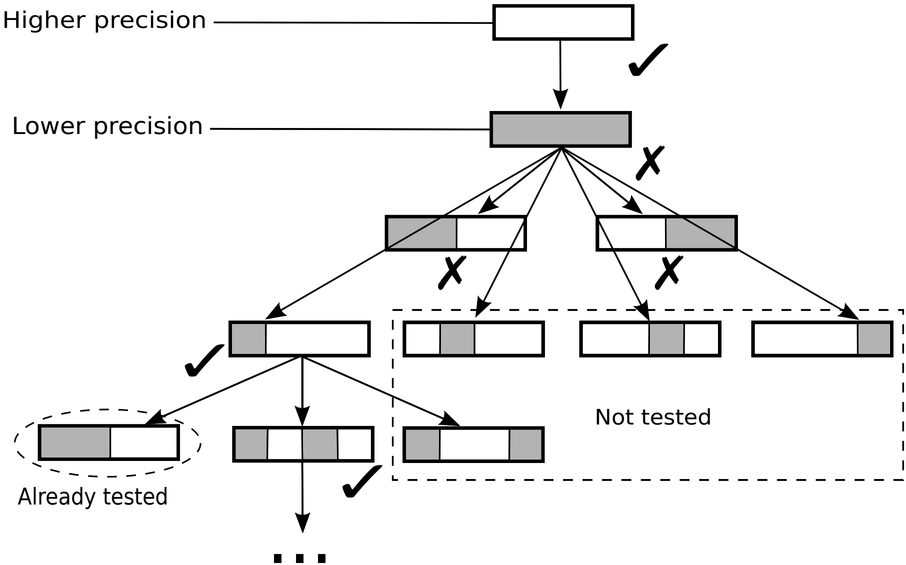
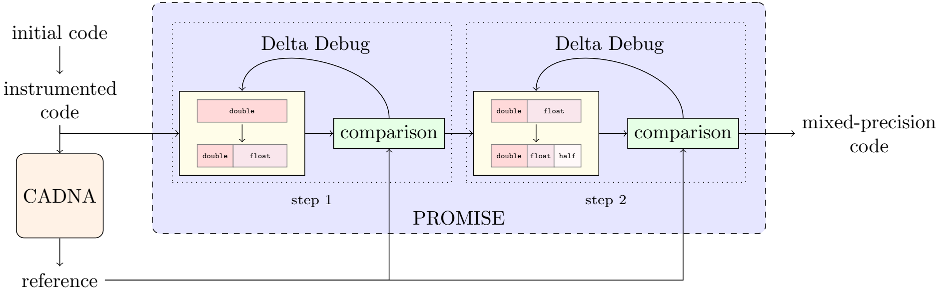


PROMISE in double, single and half precision



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

Control application

Active controller of vehicle longitudinal oscillations:

$$\left\{ \begin{array}{rcl} x(k+1) & = & Ax(k)+Bu(k) \\ y(k) & = & Cx(k)+Du(k) \end{array} \right.$$

A, B, C and D are given matrices, k is time.

Control application

Active controller of vehicle longitudinal oscillations:

$$\begin{cases} x(k+1) &= Ax(k)+Bu(k) \\ y(k) &= Cx(k)+Du(k) \end{cases}$$

After 100 iterations:

# req. digits	# exec	# half-# single-# double	time (s)
1-2	58	6-12-0	58.16
3	52	0-18-0	51.47
4	55	0-15-3	47.53
5	62	0-11-7	50.92
6	67	0-9-9	53.76
7	66	0-7-11	50.89
8	63	0-4-14	47.36
9-11	52	0-1-17	38.10

time: total execution time of PROMISE (compilations, executions, and time spent in PROMISE routines)

Active controller of vehicle longitudinal oscillations:

$$\begin{cases} x(k+1) & = & Ax(k)+Bu(k) \\ y(k) & = & Cx(k)+Du(k) \end{cases}$$

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7	66	0-7-11	50.89
8	63	0-4-14	47.36
9-11	52	0-1-17	38.10

time: total execution time of PROMISE (compilations, executions, and time spent in PROMISE routines)

MICADO: simulation of nuclear cores

code developed by EDF (French energy supplier)

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

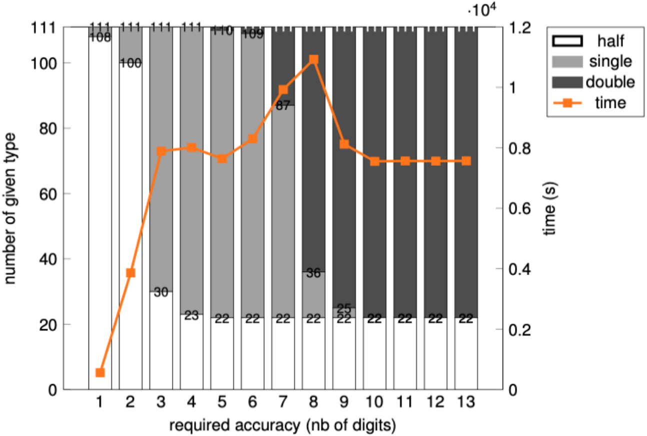
# req. digits	# single - # double	speed up	memory gain
10	32-19	1.01	1.00
8	33-18	1.01	1.01
6	38-13	1.20	1.44
5 4	51-0	1.32	1.62

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

Precision autotuning of neural networks

Generation of mixed precision C++ codes from Pytorch or Keras models

Ex: classification network for CIFAR (5 layers, 111 types to set)



Conclusion/Perspectives

To optimize precision

- numerical validation tools such as CADNA
- precision autotuning tools such as PROMISE
- mixed precision algorithms

Work in progress: extension of PROMISE to arbitrary precision

- relies on FloatX (similar to FlexFloat, completely in C++)
  `https://github.com/oprecomp/FloatX`
- From a list of numerical formats (e.g. fp64, fp32, bf16, E4M3), several Delta Debug executions identify which variables/parts can be relaxed to lower precisions

Perspectives

- extension of PROMISE to GPUs
- combination of mixed precision algorithms and floating-point autotuning

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Thank you for your attention!