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

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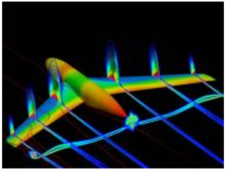
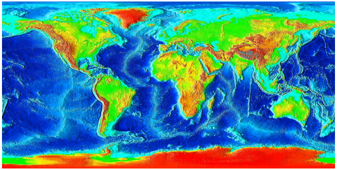
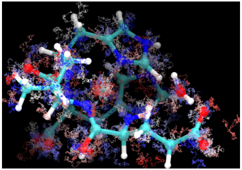
Introduction

High performance simulations required in many domains







Many efforts on performance

Exascale (10^{18} floating-point operations per second)

Each elementary operation can generate a rounding error

$\Rightarrow$ numerical validation is crucial

Introduction

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

Various floating-point formats (non-exhaustive list):

	#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

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

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

Impact of rounding errors: an example

Let $P = 333.75y^6 + x^2(11x^2y^2 - y^6 - 121y^4 - 2) + 5.5y^8 + x/(2y)$
with $x = 77617$ and $y = 33096$

[S.M. Rump, 1988]

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

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

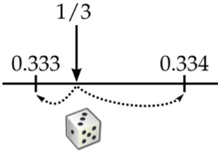
$A_1 \oplus B_1$  $\longrightarrow R_1$

$A_2 \oplus B_2$  $\longrightarrow R_2$

$A_3 \oplus B_3$  $\longrightarrow R_3$

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

- each operation executed 3 times with a random rounding mode



Discrete Stochastic Arithmetic (DSA) [Vignes'04]

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DSA

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$A_3 \oplus B_3$  $\longrightarrow R_3$

R_1 =**3.141**354786390989
R_2 =**3.143**689456834534
R_3 =**3.142**579087356598

- 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%

Discrete Stochastic Arithmetic (DSA) [Vignes'04]

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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
  ⇒ 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],...

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;
}
int main() {
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  double   x, y;
  x=10864.0; y=18817.0;
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  return 0;
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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);
  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);
  double_st x, y;
  x=10864.0; y=18817.0;
  cout«"P1="«rump(x, y)«endl;
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  cadna_end();
  return 0;
}
```

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)

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. $-\infty$)

The SAM library

www-pequan.lip6.fr/~jezequel/SAM

SAM (Stochastic Arithmetic in Multiprecision)

implements stochastic arithmetic in arbitrary precision (based on MPFR[1])
`mp_st` stochastic type

operator overloading ⇒ few modifications in user C/C++ programs

[1] www.mpfr.org

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implements stochastic arithmetic in arbitrary precision (based on MPFR[1])
`mp_st` stochastic type

operator overloading ⇒ few modifications in user C/C++ programs

- uniform precision version [Graillat & al.'11]
- mixed precision version: control of operations mixing different mantissa lengths

Ex: mp_st<23>A; mp_st<47>B; mp_st<35>C;

$$C = A \oplus B$$

35 bits   23 bits   47 bits

⇒ accuracy estimation on FPGA

[1] www.mpfr.org

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

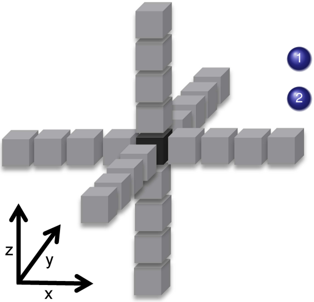
- time: order 2
- space: order p (in our case $p = 8$).

2 implementations of the finite difference scheme

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

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

where u^n_{ijk} (resp. f^n_{ik}) 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



1. nearest neighbours first
2. dimension 1, 2 then 3

Reproducibility problems

Results depend on:

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

In fp32, for $64 \times 64 \times 64$ space steps and 1000 time iterations:

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

Results computed at 3 different points

scheme	point in the space domain		
	$p_1 = (0, 19, 62)$	$p_2 = (50, 12, 2)$	$p_3 = (20, 1, 46)$
AMD Opteron CPU with gcc			
1	**-1.11**0479E+0	**5.454**238E+1	**6.1410**38E+2
2	**-1.11**0426E+0	**5.454**199E+1	**6.1410**35E+2
NVIDIA C2050 GPU with CUDA			
1	**-1.11**0204E+0	**5.454**224E+1	**6.1410**46E+2
2	**-1.10**9869E+0	**5.454**244E+1	**6.1410**47E+2
NVIDIA K20c GPU with OpenCL			
1	**-1.10**9953E+0	**5.454**218E+1	**6.1410**44E+2
2	**-1.11**1517E+0	**5.454**185E+1	**6.1410**24E+2
AMD Radeon GPU with OpenCL			
1	**-1.10**9940E+0	**5.454**317E+1	**6.1410**38E+2
2	**-1.11**0111E+0	**5.454**170E+1	**6.1410**44E+2
AMD Trinity APU with OpenCL			
1	**-1.11**0023E+0	**5.454**169E+1	**6.1410**62E+2
2	**-1.11**0113E+0	**5.454**261E+1	**6.1410**49E+2

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How to estimate the impact of rounding errors?

The wave propagation code examined with CADNA

The code is run on:

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

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

Its mean value is:

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

$\Rightarrow$ consistent with our previous observations

Instabilities detected: > 270 000 cancellations

The wave propagation code examined with CADNA

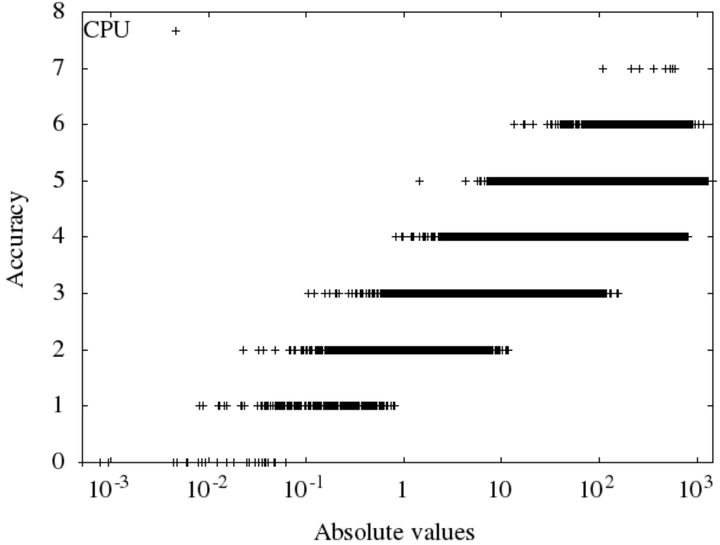
Results computed at 3 different points using scheme 1:

	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

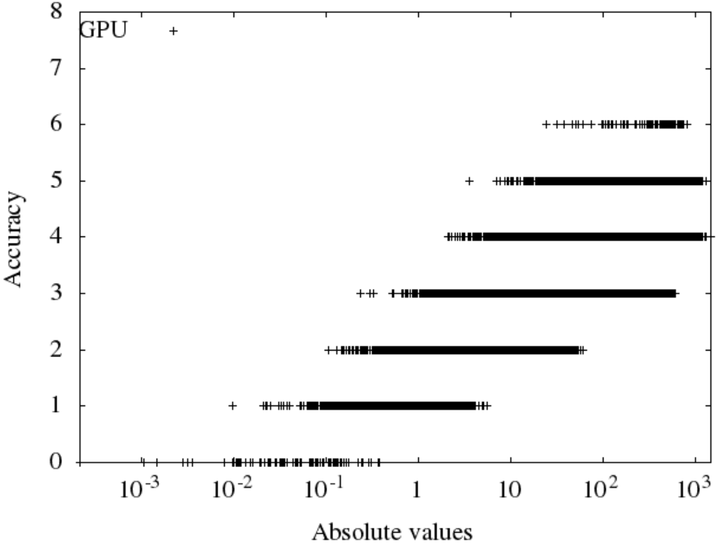
Despite differences in the estimated accuracy, the same trend can be observed on CPU and on GPU.

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

Accuracy distribution on CPU

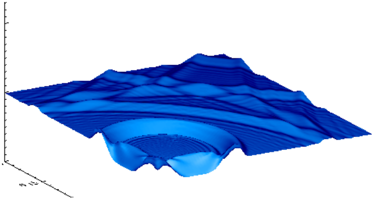


Accuracy distribution on GPU



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

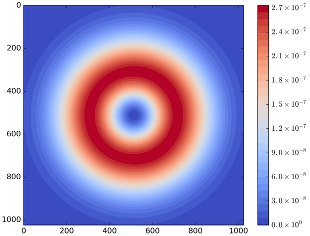
- Simulation of the evolution of water height and velocities in a 2D oceanic basin
- CUDA GPU code in double precision



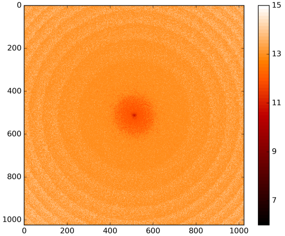
- Focusing on an eddy evolution:
  20 time steps (12 hours of simulated time)
  on a 1024 × 1024 grid

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**

Tools related to CADNA

available on `cadna.lip6.fr`

- CADNAIZER
  - automatically transforms C/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

Other numerical validation tools based on result perturbation

- VERIFICARLO [Denis & al.'16] based on LLVM
- VERROU [Févotte & al.'17] based on Valgrind, no source code modification ☺

- asynchronous approach: 1 complete run → 1 result
- several executions:
  - for rounding error analysis
  - to point out unstable tests
- no support for GPU codes.

Cost comparison

C++ arithmetic benchmarks (compute/memory bound) [Picot'18]

	3 samples w.r.t classic exec.
CADNA	$\approx$ 5 to 8
VERIFICARLO	$\approx$ 300 to 600
VERROU	$\approx$ 30

If the results accuracy is not satisfactory...

- higher precision: `single` → `double` → `quad` → arbitrary precision
  ⚠ 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]

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

- mixed precision linear algebra algorithms
  - matrix-matrix and matrix-vector multiplication
  - LU and QR matrix factorizations
  - iterative refinement
  - Krylov solvers
  - least squares problems

  survey: [Higham & Mary'22]

- precision autotuning
  transforms a code into mixed precision whatever the algorithms it implements

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
- 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
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]

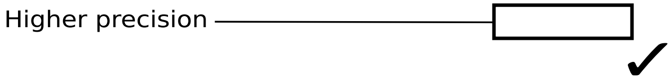
promise.lip6.fr

PROMISE

- provides a mixed precision code (half, single, double) 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.

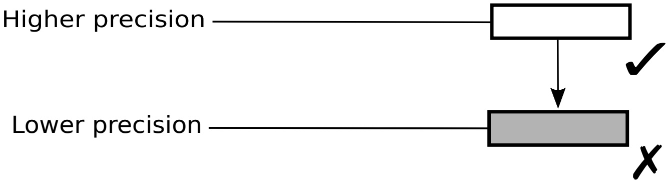
Searching for a valid configuration with 2 types

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



Searching for a valid configuration with 2 types

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



Searching for a valid configuration with 2 types

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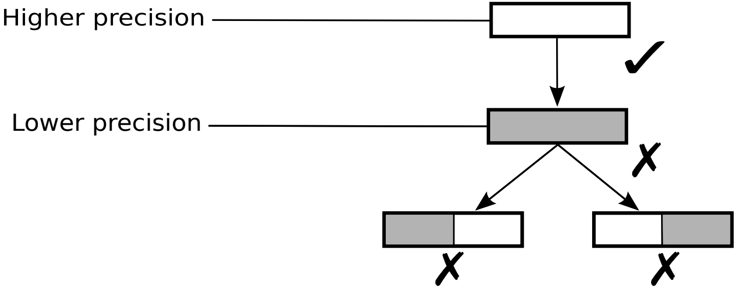
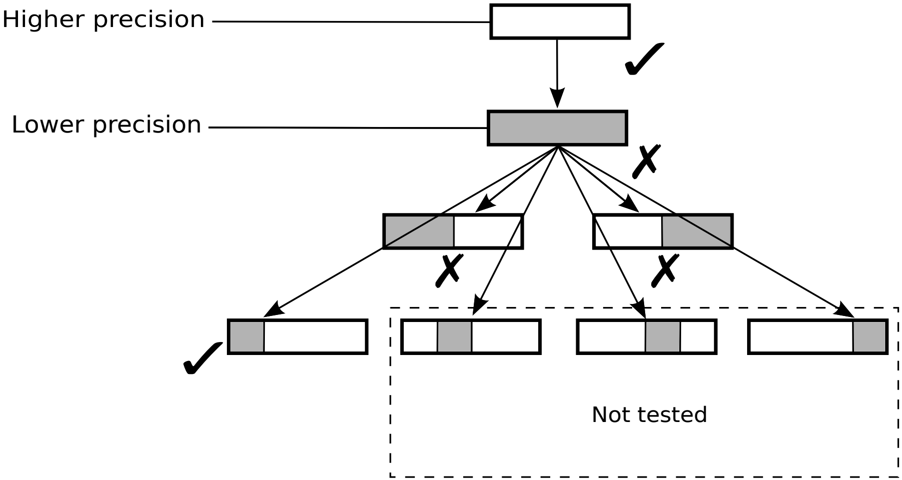


Searching for a valid configuration with 2 types

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



Searching for a valid configuration with 2 types

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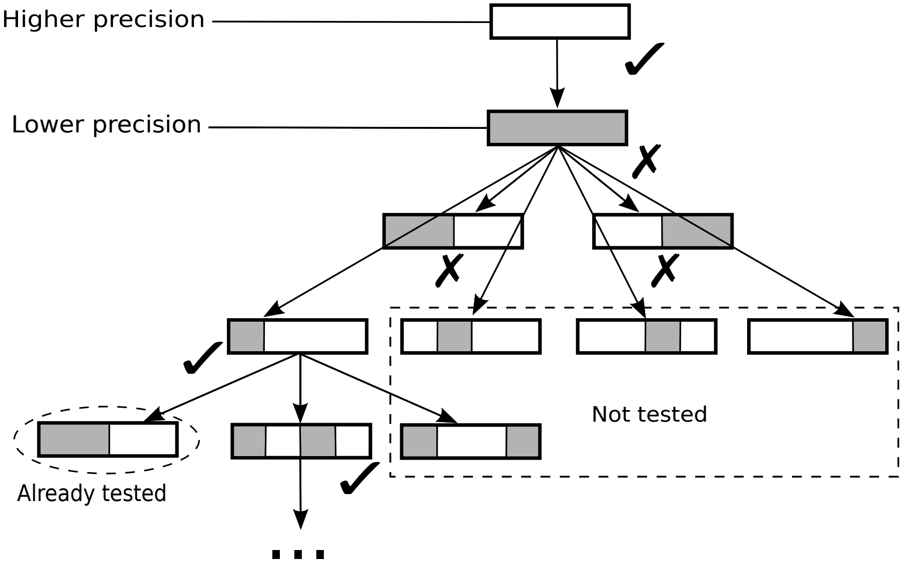
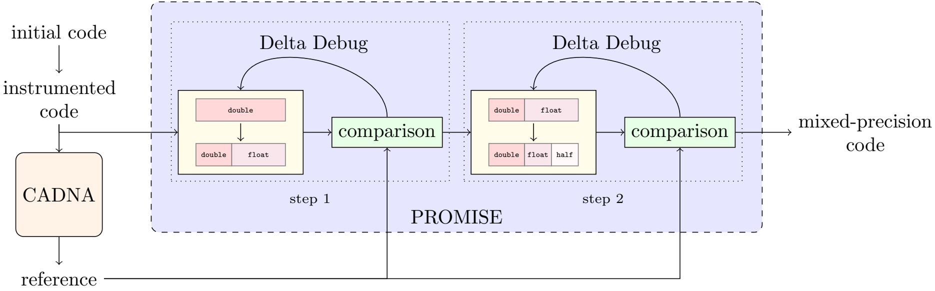


PROMISE data flow



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

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

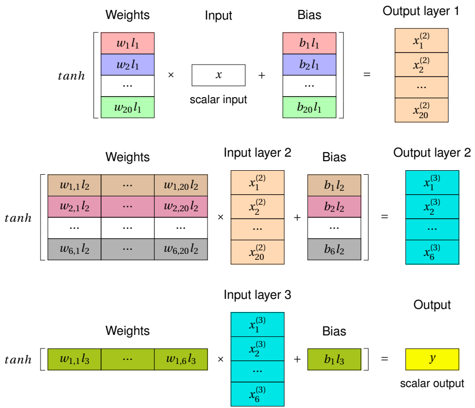
Precision autotuning of neural networks

- neural networks created and trained with Keras or PyTorch
- automatically transformed into C++ codes to be used with PROMISE

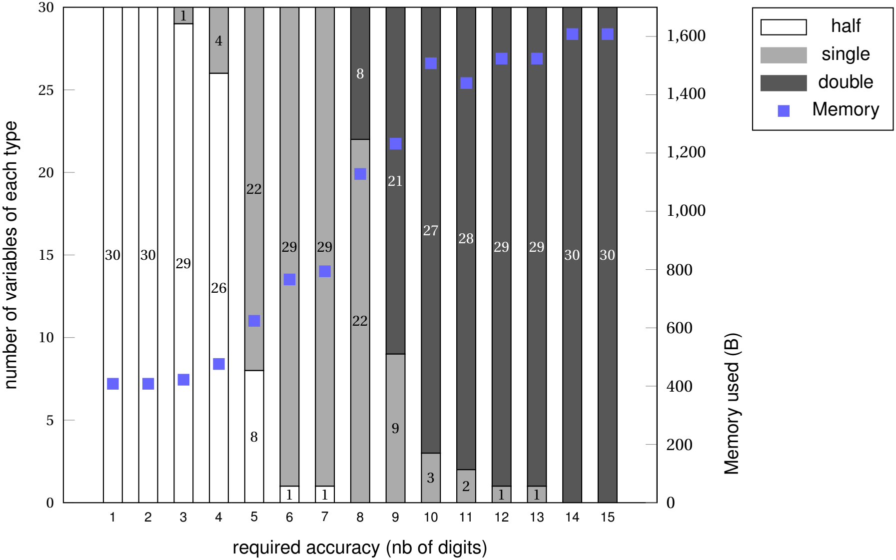
Sine NN: interpolation network approximating the sine function

- Scalar input/ouput
- 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

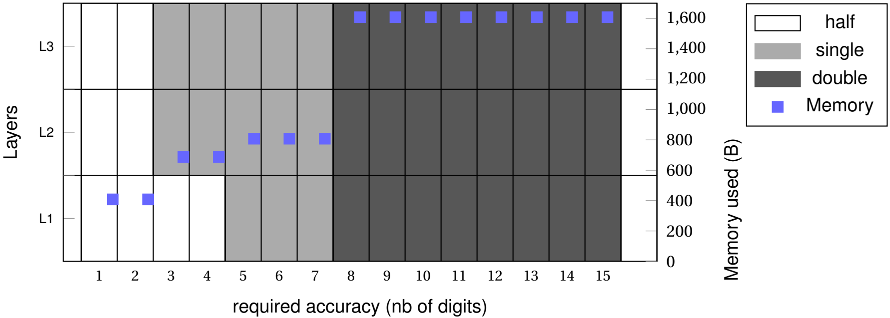
⇒ 30 types to set in total



Sine NN, one type per neuron



Sine NN, one type per layer



In this talk, input=0.5
similar trends observed with different input values

MNIST NN

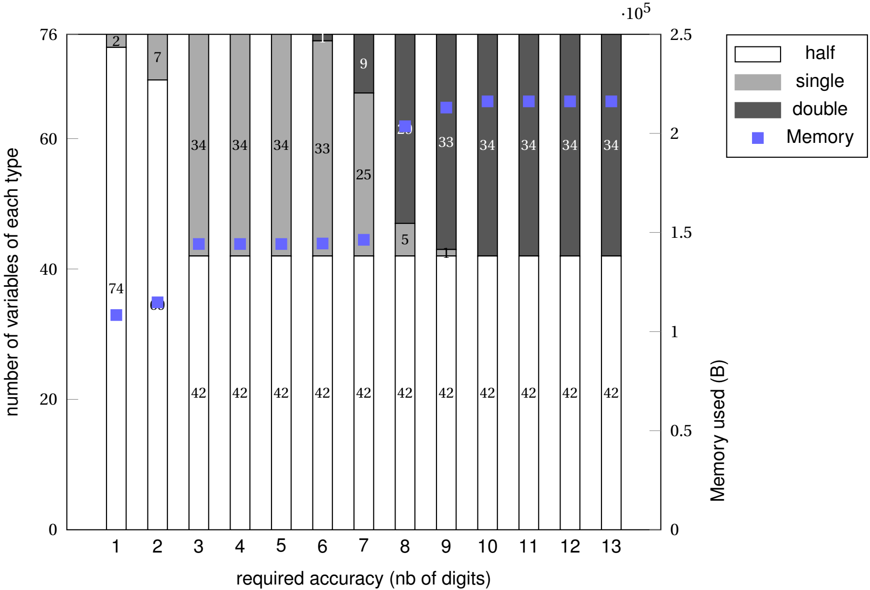
Classification of handwritten digits:

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

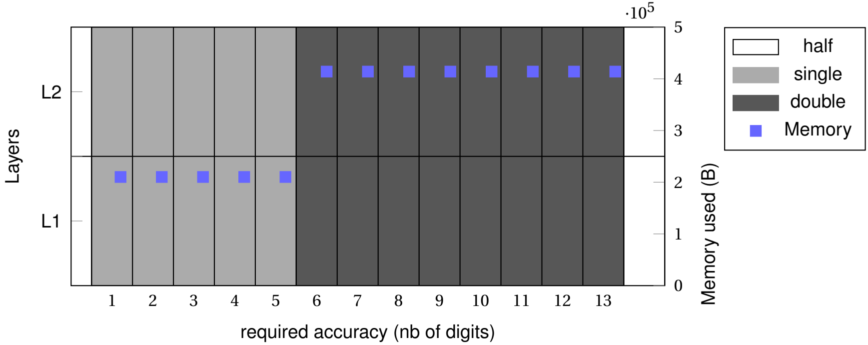
⇒ 76 types to set in total

wikipedia.org

MNIST NN, one type per neuron



MNIST NN, one type per layer



In this talk, input image test_data[61] from MNIST data base
similar trends observed with different input images

Conclusion/Perspectives

To optimize precision

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

Perspectives

- floating-point autotuning in arbitrary precision (work in progress)
- extension of PROMISE to GPUs
- combination of mixed precision algorithms and floating-point autotuning

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Thank you for your attention!