## CADNA demo

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## CADNA installation

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

```
gunzip cadna_c-3.1.3.tar.gz
tar -xvf cadna_c-3.1.3.tar
cd cadna_c-3.1.3
./configure --prefix='pwd' --enable-fortran
make install
```

Automatic detection of OpenMP, MPI. Up to 10 libraries can be created.
Ex: libcadnaC.a, libcadnaCdebug.a, libcadnaMPICforOpenMP.a, libcadnaMPICdebugforOpenMP.a, libcadnaMPIFortran.a,...

- optimized versions: inlining, -O3
- debug versions: no inlining, -O0, -g

Successfully tested with GNU (gcc, gfortran), IBM (xlc, xlf), Intel (icpc, ifort), LLVM (clang, xlflang), PGI (pgcc, pgfortran) compilers.

## Outline

## (1) CADNA installation

(2) Numerical validation of $C / C++$ codes

## (3) Numerical validation of Fortran codes

4 The CADTRACE tool

## Example 1 [s.M. Rump. 1988]

$$
\begin{aligned}
& P=333.75 y^{6}+x^{2}\left(11 x^{2} y^{2}-y^{6}-121 y^{4}-2\right)+5.5 y^{8}+x /(2 y) \\
& \text { with } x=77617 \text { and } y=33096
\end{aligned}
$$

Exact result : $P \approx-0.827396059946821368141165095479816292$
므 Execution without/with CADNA

## Example 2

The roots of the following second order equation are computed:

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

The exact values are:

- Discriminant $d=0$
- $x_{1}=x_{2}=3.5$

므 Execution without/with CADNA:

- without CADNA: wrong branching $\Rightarrow$ the result is false
- with CADNA:
if ( $d==0$.) is satisfied if $d$ is numerical noise


## Example 3

The determinant of Hilbert's matrix of size 11 defined by

$$
a_{i, j}=1 /(i+j-1)
$$

is computed without pivoting strategy.
After triangularization, the determinant is the product of the diagonal elements.

ㅁ Execution without/with CADNA

## Example 4 [J.-M. Muller, 1987]

The 25 first iterations of the following recurrent sequence are computed:

$$
U_{n+1}=111-1130 / U_{n}+3000 /\left(U_{n} * U_{n-1}\right)
$$

with $U_{0}=5.5$ and $U_{1}=61 / 11$.

The exact limit is 6 .
ㅁ Execution without/with CADNA
With CADNA, instabilities related to DSA self-validation are detected. Then, the accuracy estimation is not reliable.

## Example 5

A root of the polynomial

$$
f(x)=1.47 x^{3}+1.19 x^{2}-1.83 x+0.45
$$

is computed by Newton's method. The sequence is initialized with $x=0.5$. The iterative algorithm

$$
x_{n+1}=x_{n}-f\left(x_{n}\right) / f^{\prime}\left(x_{n}\right)
$$

is stopped by the criterion

$$
\left|x_{n}-x_{n-1}\right|<10^{-12} .
$$

ㅁ Execution without/with CADNA

## Example 5

## Without CADNA

- stopping criterion fabs $(x-y)<1 . e-12$

$$
\begin{aligned}
& x(35)=+4.285714252078272 e-01 \\
& x(36)=+4.285714252078272 e-01
\end{aligned}
$$

The stopping criterion is satisfied by chance.

## With CADNA

- stopping criterion fabs $(x-y)<1 . e-12$

$$
\begin{aligned}
& x(100)=0.4285714 \mathrm{E}+000 \\
& x(101)=0.4285714 \mathrm{E}+000
\end{aligned}
$$

if $x-y$ is numerical noise, the test is not satisfied
$\Rightarrow$ maximum number of iterations
Because of instable divisions detected by CADNA, a multiple root is suspected.

## Example 5

## With CADNA

- stopping criterion fabs $(x-y)<=1 . e-12$ or $x==y$
$x(23)=0.428571437 \mathrm{E}+000$
$x(24)=0.42857143 \mathrm{E}+000$
if $x-y$ is numerical noise, the test is satisfied.
- we simplify the faction, and so compte a simple root.
stopping criterion $\mathrm{x}==\mathrm{y}$
$x(45)=0.428571428571430 \mathrm{E}+000$
$x(46)=0.428571428571429 \mathrm{E}+000$


## Example 6

A linear system of size 4 is solved using Gaussian elimination with partial pivoting.

ㅁ Execution without/with CADNA

- Without CADNA
when $\mathrm{i}=2$, a[2] [2] is 4864.
But that value has actually no correct digits (associate exact value: 0 ). $a[2][2]$ is chosen as the pivot and leads to round-off errors in the subsequent computation.
- With CADNA

One can observe that a[2][2] has no correct digits.
The test fabsf(a[j][i])>pmax fails.
a[3] [2], that is computed accurately, is chosen as the pivot.

## Example 7

## Example created on purpose to make CADNA fail

We compute several times:

$$
\begin{aligned}
& \mathrm{x}=6.83561 \mathrm{e}+5 ; \mathrm{y}=6.83560 \mathrm{e}+5 ; \mathrm{z}=1.00000000007 ; \\
& \mathrm{r}=((\mathrm{z}-\mathrm{x})+\mathrm{y})+((\mathrm{z}-\mathrm{y})+\mathrm{x}-2) ;
\end{aligned}
$$

Exact result: $1.410^{-10}$
ㅁ Execution without/with CADNA
Without CADNA:
using IEEE double precision with rounding to nearest
$\mathrm{r}=2.32830643653870 \mathrm{E}-10$

## With CADNA:

we perform close evaluations: $((z-x)+y)$ and $((z-y)+x-2)$.
If the same rounding mode is chosen for both parts, the final result appears as exact but it is wrong.
1 case in 4 CADNA provides $0.116415321826935 \mathrm{E}-009$, otherwise @. 0

## Example with OpenMP [Eberhart et al., 2016]

The sum S of an array $A$ of size $2 n$ with $n=10^{6}$ is computed in single precision:

```
#pragma omp parallel for
for (i=0;i<2*n;i=i+2) {
    A[i+1]=(float)i+1.;
    A[i]=-(float)i;
    }
S=0.;
#pragma omp parallel for reduction(+:S) schedule(static,1)
for (i=0;i<2*n;i++)
    S=S+A[i];
```

Exact result: $S=10^{6}$
므 Execution without/with CADNA

## Two scheduling options

|  | (static) |  | (static,1) |  |
| :---: | :---: | :---: | :---: | :---: |
| \# threads | without CADNA | with CADNA | without CADNA | with CADNA |
| 1 | $1.000000 \mathrm{E}+06$ | $1.000000 \mathrm{E}+06$ | $1.000000 \mathrm{E}+06$ | $1.000000 \mathrm{E}+06$ |
| 2 | $1.000000 \mathrm{E}+06$ | $1.000000 \mathrm{E}+06$ | $1.966080 \mathrm{E}+06$ | $@ .0$ |
| 3 | $1.000000 \mathrm{E}+06$ | $1.000000 \mathrm{E}+06$ | $1.000000 \mathrm{E}+06$ | $1.000000 \mathrm{E}+06$ |
| 32 | $1.000000 \mathrm{E}+06$ | $1.000000 \mathrm{E}+06$ | $1.892352 \mathrm{E}+06$ | $@ .0$ |
| 64 | $1.000000 \mathrm{E}+06$ | $1.000000 \mathrm{E}+06$ | $1.787904 \mathrm{E}+06$ | $@ .0$ |
| 128 | $1.000000 \mathrm{E}+06$ | $1.000000 \mathrm{E}+06$ | $1.609728 \mathrm{E}+06$ | $@ .0$ |
| 239 | $1.000000 \mathrm{E}+06$ | $1.000000 \mathrm{E}+06$ | $1.000000 \mathrm{E}+06$ | $1.000000 \mathrm{E}+06$ |
| 240 | $1.000000 \mathrm{E}+06$ | $1.000000 \mathrm{E}+06$ | $1.617920 \mathrm{E}+05$ | $@ .0$ |

- (static): the loop is divided into chunks of size $2 n / T$ where $T$ is the number of threads.
Each thread has in charge contiguous elements of A and alternatively sums positive and negative values: all results are accurate.
- (static, 1 ): the chunk size is 1 .
- odd number of threads: correct result
- even number of threads: the result has no correct digits


## With (static,1) and an even number of threads

- With 2 threads:

$A:$| 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |

$\square$ thread $0 \quad \square$ thread 1
thread 0 computes $P(n)=\sum_{i=0}^{n-1}(-2 i)=-n^{2}+n$
and thread $1 Q(n)=\sum_{i=0}^{n-1}(2 i+1)=n^{2}$.
For $k=2, \ldots, n$,
$P(k)=P(k-1)-(2 k-2)=-\left((k-1)^{2}+k-1\right)-(2 k-2)$
and $Q(k)=Q(k-1)+2 k-1=(k-1)^{2}+2 k-1$.
The computation of $P(k)$ and $Q(k)$ involves values with different orders of magnitude and generates round-off errors for $k$ sufficiently high.

- With an even number of threads $>2$ : same phenomenon.

The reduction involves inaccurate results with close absolute values and different signs and thus provides numerical noise.

## With (static,1) and an odd number of threads

For example, with 3 threads:


Each thread has in charge positive and negative elements of $A$. No cancellation occurs and all results are accurately computed.

## Example with MPI [S.M. Rump, 1983]

We compute using 4 MPI processes $P=9 x^{4}-y^{4}+2 y^{2}$ with $x=10864$ and $y=18817$.

Processes 1, 2 and 3:

- compute respectively $9 x^{4},-y^{4}$ and $2 y^{2}$
- send their local result to process 0 .

Process 0 receives and sums the results.

Exact result : $P=1$.
므 Execution without/with CADNA
mpirun -np 4 exampleMPI1
mpirun -np 4 exampleMPI1_cad

## Example with MPI and OpenMP [s.M. Rump, 1983]

We compute using 4 MPI processes $P=9 x^{4}-y^{4}+2 y^{2}$ with $x=10864$ and $y=18817$.

Processes 1, 2 and 3:

- compute respectively $9 x^{4},-y^{4}$ and $2 y^{2}$ in parallel using OpenMP
- send their local result to process 0 .

Process 0 receives and sums the results.

Exact result : $P=1$.
므 Execution without/with CADNA
mpirun -np 4 exampleMPI_OMP1
mpirun -np 4 exampleMPI_OMP1_cad

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- version of CADNA written in Fortran
- CADNA in C can be used in Fortran codes thanks to Fortran/C binding Example: addition of two double_st variables (in srcFortran) in cadna_add.f90:

```
interface operator(+)
```

    module procedure add_double_st_double_st
    end interface operator (+)
    interface
    pure function cpp_add_double_st_double_st(a, b) bind(C)
                import double_st
                type(double_st), intent(in) : : a
        type(double_st), intent(in) :: b
        type(double_st) cpp_add_double_st_double_st
            end function cpp_add_double_st_double_st
    end interface
    in cadna_add_binding.cc:
double_st cpp_add_double_st_double_st( double_st \&a, double_st \&b )
\{ return $a+b ;$ \}

+ specific Fortran sources for overloading of array functions (MATMUL, SUM, PRODUCT,...)

므 Executions without/with CADNA in examplesFortran

## Outline

## (1) CADNA installation

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(3) Numerical validation of Fortran codes

4 The CADTRACE tool

## The CADTRACE tool

CADTRACE can be freely downloaded from http://cadna.lip6.fr

```
Installation
gunzip cadtrace-2.2.tar.gz
tar -xvf cadtrace-2.2.tar
cd cadtrace-2.2
./configure --prefix='pwd'
make install
```

Use gdb with the gdb_c.in file provided in the extra-files directory and generate a gdb. out file.

므 Example with a C program in the examplesC directory: gdb ex5_cad<gdb_c.in>gdb.out

To obtain a detailed list of instabilities:
cadtrace_gcc gdb.out

ㅁ Example with a Fortran program in the examplesFortran directory:
gdb ex5_cad<gdb_c.in>gdb.out
To obtain a detailed list of instabilities:
cadtrace_gcc gdb.out
You can also specify the number of function calls that generate each instability. For instance, to get 3 levels of function calls:
cadtrace_gcc -n 3 gdb.out

Remark: the cadna_enable, cadna_disable functions may help for numerical debugging.

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Thank you for your attention!

