

Verrou: A Tool to Reproduce Floating-Point-Induced Non-Reproducibilities (and help fix them)

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Industrial context – Numerical Verification In-house development of Scientific Computing Codes



Structures



Fluid dynamics



Wave propagation





Power Systems



Free surface hydraulics



Industrial context – Numerical Verification Verification & Validation



Floating-point arithmetic

- round-off errors: $a \oplus b \neq a + b$
- loss of associativity: $(a \oplus b) \oplus c \neq a \oplus (b \oplus c)$
- reproducibility issues with e.g. parallelization, vectorization, optimization...



Industrial context – Numerical Verification Verification & Validation



Quantifying numerical errors: at stake

- quality of produced results (accuracy, reproducibility...)
- efficient use of resources (development & computing time)



Industrial context – Numerical Verification

Example: performances of an optimization problem

Initial problem formulation

$$\max_{\boldsymbol{p}, \boldsymbol{v}} \sum_{t \in T} \sum_{i \in I} \lambda_t \boldsymbol{p}_t^i + \sum_{r \in R} \omega_r \left(\boldsymbol{v}_t^r - \boldsymbol{V}_0^r - \sum_{t \in T} \boldsymbol{\Gamma}_t^r \right)$$

Objective functional computation

$$\sum_{t \in T} \sum_{i \in I} \lambda_t p_t^i + \sum_{r \in R} \omega_r v_t^r$$
$$- \sum_{r \in R} \omega_r \left(V_0^r + \sum_{t \in T} \Gamma_t^r \right)$$

1534019.677371745

-1534019.677282780



Industrial context – Numerical Verification Example: performances of an optimization problem

Proposed re-formulation

$$\left[\max_{\boldsymbol{p}, \boldsymbol{v}} \sum_{t \in T} \sum_{i \in I} \lambda_t \boldsymbol{p}_t^i + \sum_{r \in R} \omega_r \boldsymbol{v}_t^r\right] - \sum_{r \in R} \omega_r \left(V_0^r + \sum_{t \in T} \Gamma_t^r \right)$$

Objective functional computation

$$\sum_{t \in T} \sum_{i \in I} \lambda_t p_t^i + \sum_{r \in R} \omega_r v_t^r$$
$$- \sum_{r \in R} \omega_r \left(V_0^r + \sum_{t \in T} \Gamma_t^r \right)$$

1534019.677371745

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Industrial context – Numerical Verification

Example: performances of an optimization problem



Industrial context – Numerical Verification Objectives / presentation outline

Diagnostics

- verify a code / show the presence of FP-related errors
- quantify the magnitude of issues

Debugging

- Iocate the origin of FP-related issues in the source code
 - unstable algorithms
 - unstable tests
- track the origin of issues during program execution
 - context of calls
 - temporal information (e.g. iteration number...)

Optimization

use mixed-precision implementations





Available on github (latest version: v2.1.0) http://github.com/edf-hpc/verrou

Documentation: http://edf-hpc.github.io/verrou/vr-manual.html



Industrial context – Numerical Verification

Analyse dynamique du binaire avec Valgrind

\$ valgrind --tool=verrou [VERROU_ARGS] PROGRAM [ARGS...]





Diagnostics: detect and assess instabilities Verrou back-end: random rounding

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IEEE-754: nearest rounding mode





Diagnostics: detect and assess instabilities

Verrou back-end: random rounding

CESTAC/MCA: random rounding mode --rounding-mode=random

- [1] J. Vignes, "A stochastic arithmetic for reliable scientific computation," *Mathematics and Computers in Simulation*, vol. 35, no. 3, 1993.
- [2] J.-L. Lamotte, J.-M. Chesneaux and F. Jézéquel, "CADNA_C: A version of CADNA for use with C or C++ programs", Computer Physics Communications, vol. 181, no. 11, 2010.
- [3] D. Stott Parker, "Monte Carlo Arithmetic: exploiting randomness in floating-point arithmetic", Univ. California, 1997.



Diagnostics: detect and assess instabilities

Verrou back-end: random rounding



- J. Vignes, "A stochastic arithmetic for reliable scientific computation," *Mathematics and Computers in Simulation*, vol. 35, no. 3, 1993.
- [2] J.-L. Lamotte, J.-M. Chesneaux and F. Jézéquel, "CADNA_C: A version of CADNA for use with C or C++ programs", Computer Physics Communications, vol. 181, no. 11, 2010.
- [3] D. Stott Parker, "Monte Carlo Arithmetic: exploiting randomness in floating-point arithmetic", Univ. California, 1997.



Diagnostics: detect and assess instabilities Code_aster

Mechanics

- Seismic
- Acoustic
- Thermo-mechanics

$\mathsf{Code}_\mathsf{Aster}$

- 1.2M code lines
- Fortran 90, C, Python
- thousands of test cases
- Large number of dependencies :
 - ► Linear solvers (MUMPS...)
 - Mesh generator and partitioning tools (Metis, Scotch...)

Goals

understand the non-reproducibility between test computers





Diagnostics: detect and assess instabilities

Using Verrou and Random Rounding

Test	
case	nearest
ssls108i	OK
ssls108j	OK
ssls108k	OK
ssls1081	OK
sdnl112a	OK
ssnp130a	OK
ssnp130b	OK
ssnp130c	OK
ssnp130d	OK



Diagnostics: detect and assess instabilities

Using Verrou and Random Rounding

Test		
case	nearest	rnd_1
ssls108i	OK	OK
ssls108j	OK	OK
ssls108k	OK	OK
ssls1081	OK	OK
sdnl112a	OK	KO
ssnp130a	OK	OK
ssnp130b	OK	OK
ssnp130c	OK	OK
ssnp130d	OK	OK



Diagnostics: detect and assess instabilities Using Verrou and Random Rounding

Test Status rnd1 rnd_2 rnd_3 nearest case ssls108i OK OK OK 0K OK 0K 0K OK ssls108j ssls108k OK 0K OK 0K ssls1081 OK 0K OK 0K sdnl112a OK KO KO KO OK OK OK 0K ssnp130a 0K ssnp130b OK 0K OK OK 0K ssnp130c OK OK ssnp130d OK OK OK **OK** 10 minutes 20 minutes each (72 test cases)



Diagnostics: detect and assess instabilities Using Verrou and Random Rounding

Test	Status				# common decimal digits
case	nearest	rnd_1	rnd_2	rnd_3	$C(rnd_1,rnd_2,rnd_3)$
ssls108i	OK	OK	OK	OK	10
ssls108j	OK	OK	OK	OK	10
ssls108k	OK	OK	OK	OK	10
ssls1081	OK	OK	OK	OK	9
sdnl112a	OK	KO	KO	KO	3
ssnp130a	OK	OK	OK	OK	9
ssnp130b	OK	OK	OK	OK	9
ssnp130c	OK	OK	OK	OK	9
ssnp130d	OK	OK	OK	OK	9
			\uparrow	(3 samples \rightarrow lower bound fo 66% of random runs with	
10 minutes		20 m	ninutes	each	66% confidence)
(72 test cases)					



Debugging: locate issues in the source code

Using code coverage comparison: code aster (test-cas

```
IEEE-754 coverage
120:subroutine fun1(area, a1, a2, n)
       implicit none
 -: integer :: n
 -: real(kind=8) :: area, a1, a2
120: if (a1 .eq. a2) then
13:
            area = a1
       else
 -5
107:
            if (n .lt. 2) then
107:
               area = (a2-a1) / (log(a2)-log(a1))
### :
            else if (n .eq.2) then
               area = sqrt (a1*a2)
###:
            else
 - 5
             1 . . .
###:
            endif
 - 1
        endif
  -5^{\circ}
120:end subroutine
```



Debugging: locate issues in the source code

Using code coverage comparison: code_aster (test-case sdnl112a)

IEEE-75	4 coverage
120:sub	routine fun1(area, a1, a2, n)
- (implicit none
- (integer :: n
- (real(kind=8) :: area, a1, a2
120:	if (a1 .eq. a2) then
13:	area = a1
- (else
107 :	if (n .lt. 2) then
107 :	area = (a2-a1) / (log(a2)-log(a1))
###:	else if (n .eq.2) then
###:	area = sqrt (a1*a2)
- (else
###:	1
- :	endif
- (endif
120:end	subroutine

Stochast 120:subi	ic Arithmetic coverage coutine fun1(area, a1,
- :	implicit none
- (integer :: n
- (real(kind=8) :: area,
120:	if (al .eq. a2) then
4 :	area = a1
- (else
116:	if (n .lt. 2) then
116:	area = (a2-a1)
###:	else if (n .eq.2)
###:	area = sqrt (a
- (else
###:	1
- (endif
- (endif
120:end	subroutine



log.L volum2 bilpla_ ecrval print plath classer_groupes_ etupla_ couhyd_pi_ ecrplr_ imovi resopt_ getgrp_marginal_ ecrpla fin_exec_main_ decopt_pi_ paraend resopt_cnt_zones_ apstop ihyd_ impression_info_ coupla gere_print_plath_ log thepla_ coutot iprit

.../aster.release .../aster.release

- Delta-Debugging [A. Zeller, 1999]
- relies on ability to restrict the scope of instrumentation/perturbations induced by Verrou





log.L # volum2 # bilpla_ # ecrval # print plath # classer_groupes_ # etupla_ # couhyd_pi_ # ecrplr_ # imovi # resopt_ # getgrp_marginal_ # ecrpla # fin_exec_main_ # decopt_pi_ # paraend_ # resopt_cnt_zones_ # apstop_ # ihyd_ # impression_info_ # coupla # gere_print_plath_ # log # thepla_ # coutot_ # iprit_

.../aster.release .../aster.release

- Delta-Debugging [A. Zeller, 1999]
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Х



log.L .../aster.release # volum2 .../aster.release # bilpla_ .../aster.release # ecrval .../aster.release .../aster.release # print plath # classer_groupes_ .../aster.release # etupla_ .../aster.release # couhyd_pi_ .../aster.release # ecrplr_ .../aster.release # imovi .../aster.release # resopt_ .../aster.release .../aster.release # getgrp_marginal_ # ecrpla .../aster.release fin_exec_main_ .../aster.release decopt_pi_ .../aster.release paraend .../aster.release resopt_cnt_zones_ .../aster.release apstop .../aster.release ihyd_ .../aster.release impression_info_ .../aster.release coupla .../aster.release gere_print_plath_ .../aster.release .../aster.release log .../aster.release thepla_ coutot_ .../aster.release iprit .../aster.release

- Delta-Debugging [A. Zeller, 1999]
- relies on ability to restrict the scope of instrumentation/perturbations induced by Verrou

\rightarrow ×



- # log.L # volum2 # bilpla_ # ecrval # print plath # classer_groupes_ # etupla_ couhyd_pi_ ecrplr_ imovi resopt_ getgrp_marginal_ ecrpla fin_exec_main_ decopt_pi_ paraend_ resopt_cnt_zones_ apstop ihyd_ impression_info_ coupla gere_print_plath_ log thepla_ coutot iprit
 - .../aster.release .../aster.release

- Delta-Debugging [A. Zeller, 1999]
- relies on ability to restrict the scope of instrumentation/perturbations induced by Verrou

\rightarrow \checkmark



log.L	/a
volum2_	/a
bilpla_	/a
ecrval_	/a
print_plath_	/a
classer_groupes_	/a
etupla_	/a
<pre># couhyd_pi_</pre>	/a
<pre># ecrplr_</pre>	/a
# imovi_	/a
<pre># resopt_</pre>	/a
<pre># getgrp_marginal_</pre>	/a
<pre># ecrpla_</pre>	/a
fin_exec_main_	/a
decopt_pi_	/a
paraend_	/a
resopt_cnt_zones_	/a
apstop_	/a
ihyd_	/a
impression_info_	/a
coupla_	/a
gere_print_plath_	/a
log	/a
thepla_	/a
coutot_	/a
iprit	/a

ster.release ster.release

- Delta-Debugging [A. Zeller, 1999]
- relies on ability to restrict the scope of instrumentation/perturbations induced by Verrou

\rightarrow ×



log.L volum2 bilpla_ ecrval print plath classer_groupes_ etupla_ # couhyd_pi_ ecrplr_ imovi resopt_ getgrp_marginal_ ecrpla fin_exec_main_ # decopt_pi_ paraend resopt_cnt_zones_ apstop_ # ihyd_ impression_info_ coupla gere_print_plath_ log thepla_ # coutot_ # iprit

.../aster.release .../aster.release

- Delta-Debugging [A. Zeller, 1999]
- relies on ability to restrict the scope of instrumentation/perturbations induced by Verrou

- Inputs :
 - run script
 - comparison script
- Output:
 - "unstable" code parts
- Also works at the source line granularity:
 - if the code was compiled with -g

13/17 **CODE**

Debugging: locate issues in the source code Delta-Debugging on code aster (test-case sdn1112a)

```
do 60 jvec = 1, nbvect
          do 30 \ k = 1, neq
              vectmp(k)=vect(k, jvec)
30
          continue
          if (prepos) call mrconl('DIVI', lmat, 0, 'R', vectmp,1)
          xsol(1, jvec) = xsol(1, jvec) + zr(jvalms-1+1) * vectmp(1)
          do 50 ilig = 2, neg
              kdeb=smdi(ilig-1)+1
              kfin=smdi(ilig)-1
              do 40 \text{ ki} = \text{kdeb}, kfin
                  icol=smhc(ki)
                  xsol(ilig,jvec)=xsol(ilig,jvec) + zr(jvalmi-1+ki) * vectmp(jcol)
                  xsol(jcol,jvec)=xsol(jcol,jvec) + zr(jvalms-1+ki) * vectmp(ilig)
40
              continue
              xsol(ilig, jvec)=xsol(ilig, jvec) + zr(jvalms+kfin) * vectmp(ilig)
50
          continue
          if (prepos) call mrconl('DIVI', lmat, 0, 'R', xsol(1, jvec),1)
60
       continue
```



Optimization for mixed precision

Verrou back-end: precision reduction

- All high-precision values are cast to single precision before performing arithmetic operations
 - emulates the use of low-precision arithmetic
 - ... but not the performance boost.

Currently implemented only for double-single (--rounding-mode=float)

- can be generalized to all precision reductions (e.g single \rightarrow half)
- can not emulate higher precision (memory problem)

Can be combined with Delta-Debugging
 find which code parts can be downgraded to lower precision

 A. Dawson and P. D. Düben, "rpe v5: an emulator for reduced floating-point precision in large numerical simulations", Geoscientific Model Development, 2017.



Wrap-up Verrou as a tool to help with FP issues

Diagnostics

☆ show the presence of FP-related errors

送 quantify the magnitude of issues

(random-rounding back-end) (post-processing)

Debugging

 $\stackrel{\scriptstyle{\scriptstyle{\leftrightarrow}}}{\simeq}$ locate the origin of FP-related issues in the source code

- -☆- unstable algorithms
- 送 unstable tests

(Delta-Debugging) (code coverage analysis)

\bigcirc track the origin of issues during program execution

- context of calls
- temporal information (e.g. iteration number...)

Optimization

O emulate mixed-precision implementations

• re-use debugging features

(reduced precision back-end)

(Delta-Debugging)



Outlooks

- Verrou is no silver bullet
 - multiply techniques & tools

Interflop (toolbox)

Common interface for Verificarlo & Verrou (and anyone interested!)

- share Stochastic Arithmetic back-ends
- share accompanying tools (Delta-Debugging...)
- improve performance of instrumentation front-ends

Interflop (consortium)

Explore different analysis methods and the links between them

17/17

- Stochastic Arithmetic
- Interval Arithmetic & Affine Forms



Thank you ! Questions ?

Get Verrou on github: http://github.com/edf-hpc/verrou

Documentation: http://edf-hpc.github.io/verrou/vr-manual.html



Relevant references I

- Jean-Marie Chesneaux and Jean Vignes, *On the robustness of the cestac method*, C. R. Acad.Sci. Paris **1** (1988), 855–860.
- A. Dawson and P. D. Düben, rpe v5: an emulator for reduced floating-point precision in large numerical simulations, Geoscientific Model Development 10 (2017), no. 6, 2221–2230.
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- François Févotte and Bruno Lathuilière, VERROU: Assessing Floating-Point Accuracy Without Recompiling, https://hal.archives-ouvertes.fr/hal-01383417, October 2016.



Relevant references II

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- Stef Graillat, Fabienne Jézéquel, and Romain Picot, Numerical validation of compensated algorithms with stochastic arithmetic, Applied Mathematics and Computation 329 (2018), 339 – 363.
- Fabienne Jézéquel, Jean-Marie Chesneaux, and Jean-Luc Lamotte, A new version of the CADNA library for estimating round-off error propagation in Fortran programs, Computer Physics Communications 181 (2010), no. 11, 1927–1928.
- William Kahan, How futile are mindless assessments of roundoff in floating-point computations?, https://people.eecs.berkeley.edu/~wkahan/Mindless.pdf, 2006.



Relevant references III

- Jean-Luc Lamotte, Jean-Marie Chesneaux, and Fabienne Jézéquel, CADNA_C: A version of CADNA for use with C or C++ programs, Computer Physics Communications 181 (2010), no. 11, 1925–1926.
- Devan Sohier, Pablo De Oliveira Castro, François Févotte, Bruno Lathuilière, Eric Petit, and Olivier Jamond, Confidence Intervals for Stochastic Arithmetic, preprint, https://hal.archives-ouvertes.fr/hal-01827319.
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- Jean Vignes, A stochastic arithmetic for reliable scientific computation, Mathematics and Computers in Simulation **35** (1993), 233–261.
 - Andreas Zeller, Yesterday, My Program Worked. Today, It Does Not. Why?, SIGSOFT Softw. Eng. Notes 24 (1999), no. 6, 253–267.





Annexes



Case study on ACTS: emulation of reduced precision + NaN detection

<pre>\$ valgrindtool=verrourounding-mode=floatexclude=excludes.exdemangle=notrace-children=yesnum-cal > ctest -V -R "BFieldMabUtils"</pre>	lers=50 ∖
· []	
==1863== NaN:	
==1863== at 0x5847E7F: _ZN5Eigen8internal4pmulIDv2_dEET_RKS3_S5_ (emmintrin.h:271)	
==1863== by 0x5858570: _ZNK5Eigen8internal17scalar_product_opIddE8packet0pIDv2_dEEKT_RS6_S7_ (BinaryFunctors.h	:89)
== 1863== by 0x59A31C9: _ZNK6Eigen8internal16binary_evaluatorINS_13CwiseBinaryOpINSO_17scalar_product_opIddEEXN CwiseBullarvOpINSO_18scalar_constant_opIdEEXNS_6MatrixIdLi2ELi1ELi0ELi2ELi1EEEEESA_EENS	S_14 0 10
IndexBasedESE ddB6packetILi16EDv2 dET0 11 (CoreEvaluators.h:727)	
E de la contra de la	
==1863== by 0x58DE2D4: _ZN5Eigen6MatrixIdLi2ELi1ELi0ELi2ELi1EEaSINS_13CwiseBinaryOpINS_8internal13scalar_sum_o; EEKN53_IN54_17s calar_product_opIddEEKNS_14CviseMullaryOpIN54_18scalar_constant_opIdEEK S SC EESC EEERSIS RKNS 90enseBaseIT EE (Matrix h:225)	pIdd 1_EE
==1863== by 0x5BDAD82: _ZN4Acts6detail16interpolate_implIN5Eigen6MatrixIdLi2ELi1ELi0ELi2ELi1EEES4_St5arrayIdLm	2EES
<pre>c_lmibLm#bbs7ubbsA54_kK50_55_L54_lm#bb (interpolation_impl.hppilo3) ==1863== by 0x5805988: _ZM4AtsiinterpolatiOHSEigen6MatriidLi2ELi1ELi0ELi2ELi1EEELm4ES3_st5arrayIdLm2EES5_vE. KT1_RKT2_RKT3_RK54_156_XT0_EE (interpolation.hppi96)</pre>	ET_R
E1	
== 1863== by 0x4F6D54: _ZNK4Acts2iInterpolatedBFieldNapiiFieldNapperILj2ELj2EE8getFieldERKN5Eigen6MatrixIdLi3E. i0ELi3ELi1EEE (InterpolatedBFieldNap.hpp:166)	Li 1EL
==1863== by 0x477030: _ZN4Acts4Test15bfield_creation1itest_methodEv (BFieldMapUtilsTests.cpp:88)	
==1863== by 0x474767: _ZN4Acts4TestL23bfield_creation_invokerEv (BFieldMapUtilsTests.cpp:25)	
==1863== by 0x549B9B:ZN5boost6detail8function22void_function_invoker0IPFvvEvE6invokeERN51_15function_buffer	E (fu
<pre>nction_template.hpp:118)</pre>	
[]	
==1863== by 0x43F2FE: _ZN5boost9unit_test9framework3runEmb (framework.ipp:1629)	
==1863== by 0x463F10:ZN5boost9unit_test14unit_test_mainEPFPNS0_10test_suiteEiPPcEiS4_ (unit_test_main.ipp:20	47)
==1863== by 0x4648CE: main (unit_test_main.ipp:303)	
[]	
Running 12 test cases	
acts-core/Tests/Utilities/BFieldMapUtilsTests.cpp(105): error: in "bfield_creation": difference{-nan} between	
value2_rz.perp() {-nan} and bField2_rz.perp() {8} exceeds ie-09%	



V&V process: ad-hoc numerical instability detection methods



▶ Idea: measure the sensitivity of the results w.r.t "neutral" parameters
 ☆ easy to do
 ⇒ ad hoc, no localization



V&V process: ad-hoc numerical instability detection methods





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Example 1: failing computation in free surface hydraulics (Telemac 2D)





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Example 1: failing computation in free surface hydraulics (Telemac 2D)





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Example 1: failing computation in free surface hydraulics (Telemac 2D)





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