Parallel Stochastic Simulations "Reproductibles" ?

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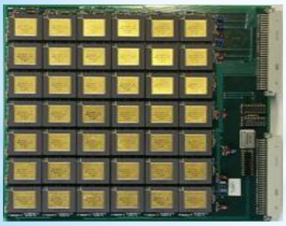
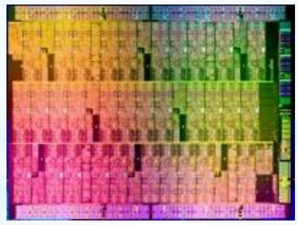
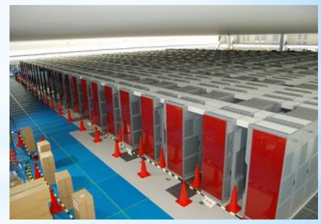
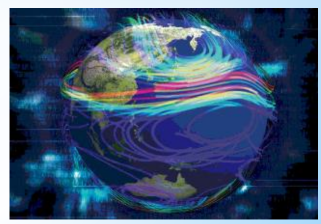
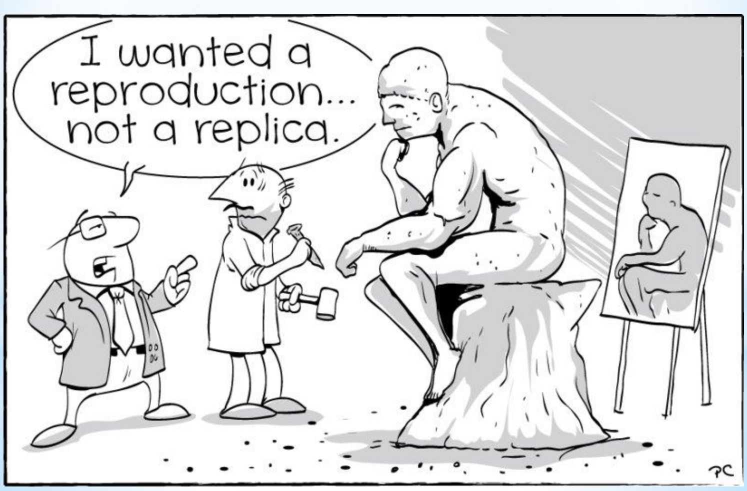




REPRODUCIBILITY BEGINNER's



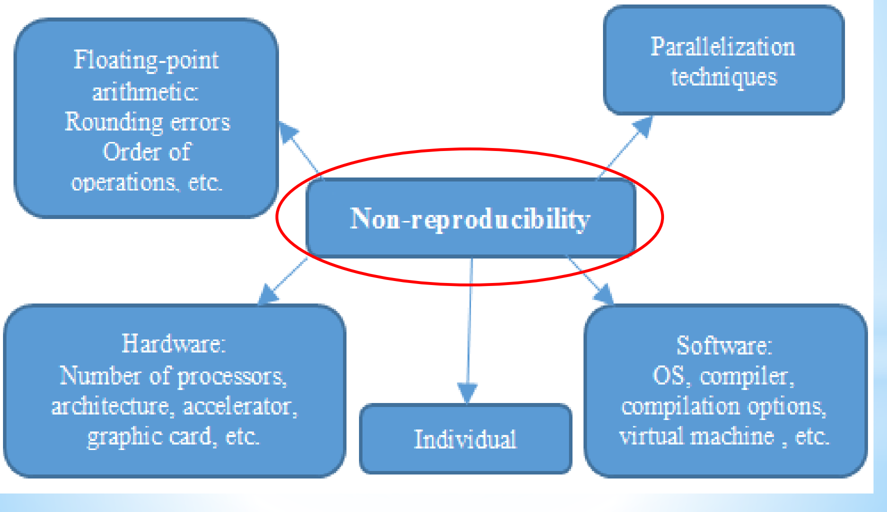
Reproducibility ? (defn.)

- In Fomel and Claerbout 2009:
  - ✓ Reproducibility **often means replication** depending on scientists

- In Drummond 2009[1]:
  - ✓ "*Reproducibility* ***requires changes; replicability avoids them***"
- In Demmel and Nguyen 2013
  - ✓ "*Reproducibility, i.e.* ***getting bitwise identical results from run to run***"
- In Revol and Théveny 2013.
  - ✓ "*What is called numerical reproducibility is the problem of getting the same result when the scientific computation is run several times, either on the same machine or on different machines, with different numbers of processing units, types, execution environments, computational loads, etc.*"

1: http://www.site.uottawa.ca/ICML09WS/papers/w2.pdf

Some Reasons for numerical reproducibility failures



Parallel Stochastic Simulations Various requirements…

- Easier if they fit with the independent bag-of-work paradigm.
  - Such stochastic simulations can easily tolerate a loss of jobs, if hopefully enough jobs finish for the final statistics..
- Must use "independent" Parallel random streams.
  - Statuses should be small and fast to store at Exascale (Original MT – 6Kb status – MRG32K3a 6 integers)
- Should fit with **different distributed computing platforms**
  - Using regular processors
  - Using hardware accelerators (GP-GPUs, Intel Phi…)

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Aim: Repeatability of parallel stochastic simulations

Remember that a stochastic program is « deterministic » if we use (initialize and parallelize) correctly the pseudo-random number.

1. A process or object oriented approach has to be chosen for every stochastic objects which has its own random stream.
2. Select a modern and statistically sound generators according to the most stringent testing battery (TestU01);
3. Select a fine parallelization technique adapted to the selected generator,
4. The **simulation must first be designed as a sequential program which would emulate parallelism**: this sequential execution – with a compiler disabling of "out of order" execution will be the reference to compare parallel and sequential execution at small scales on the same node.
5. Externalize, sort or give IDs to the results for reduction in order to keep the execution order or use compensated algorithms

[Hill 2015] : Hill D., "Parallel Random Numbers, Simulation, Science and reproducibility". IEEE/AIP - Computing in Science and Engineering, vol. 17, no 4, 2015, pp. 66-71.

An object-oriented approach?

A system being of collection of interacting "objects" (dictionary definition) – a simulation will make all those objects evolve during the simulation time with a precise modeling goal.

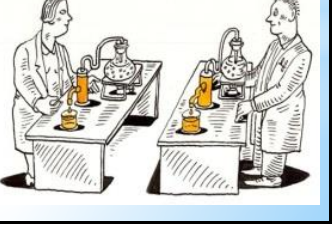
- Assign an « independent » random stream to each stochastic object of the simulation.
- Each object (for instance a particle) must have its own reproducible random stream.
- An object could also encapsulate a random variate used at some points of the simulation. Every random variate could also have their own random stream.

[Hill 1996] : HILL D., "Object-oriented Analysis and Simulation", Addison-Wesley, 1996, 291 p.

Back to basics for stochastic simulations Repeatable Par.Rand.Num.Generators

Quick check with some **top PRNGs** used with different execution context (hardware, operating systems, compilers…

1. Use exactly the same inputs
2. Execute on various environments
3. Compare our outputs with author's outputs (from publications or given files)



Reproducing results - portability 1/4

- Errors found:
  - for different hardware,
  - different operating systems,
  - different compilers.

Table 3: Testing of reproducibility for 7 different PRNGs (MT19937 with 2 versions, TinyMT with 2 versions, MRG32k3a, WELL512, MLFG64) performed on 5 different processors (Intel E5-2650v2, Intel E5-2687W, Core 2 Duo T7100, AMD 6272 Opteron, Core i7-4800MQ) with different compilers (gcc, icc, lcc, open64, MinGW, Cygwin) were tested.

Generator	**E5-2650v2**		**E5-2687W**		**Core 2 Duo T7100**		**AMD Opteron (TM) 6272**		**Core i7-4800MQ**			
	gcc	**icc**	**gcc**	**icc**	**gcc**	**open64**	**gcc**	**open64**	**Cygwin**	**MinGW**	**lcc**	
											lc	**lc64**
MT19937	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
MT19937_64	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
TinyMT_32	Yes	Yes	Yes	Yes	Yes	NO	Yes	Yes	Yes	Yes	Yes	Yes
TinyMT_64	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	NO	NO	Yes
MRG32K3a	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
WELL512a	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
MLFG_64	Yes	Yes	Yes	Yes	N/a	N/a	Yes	Yes	Yes	Yes	Yes	Yes

Reproducing results - portability 2/4

- Errors found:
  - Different Compilers (2 cases)
  - With Identical Hardware (2 cases)
  - Operating Systems (2 cases)

Table 4: Results for TinyMT_32 PRNG on Core 2 Duo T7100 running Ubuntu-13.04 with open64-i386

Expected results CHECK32.OUT.TXT	**Results obtained with Open64 i386**
0.5714423	0.5714422
0.7421532	0.7421533
0.6638085	0.6638086
0.4334422	0.4334421
0.1254190	0.1254189
0.4688578	0.4688579
0.2675911	0.2675910
0.1784127	0.1784128

Table 5: Results for TinyMT_64 PRNG on Core i7-4800MQ running Windows 7 with MinGW

Expected results CHECK64.OUT.TXT	**Results obtained with MinGW gcc**
1.152012609994736	1.152012609994737
1.363201836673650	1.363201836673651
1.218170930629463	1.218170930629464

Reproducing results - portability 3/4

- Errors found (compiler 32 vs 64 bits versions):
  Problems Encountered With 32 And 64 Bits Architecture For The Same Compiler (lcc compiler 32 bits - ok for 64 bits)

Table 6: Results for TinyMT_64 PRNG on Core i7-4800MQ running Windows 7 with lc 32 bits

Expected results CHECK64.OUT.TXT	Results obtained with lc 32 bits compiler
0.125567123229521	0.514472427354387
1.437679237017648	1.386730269781771
0.231189305675805	0.112526841009551
0.777528512172794	0.197121666699821

Reproducing results - portability 4/4

- Errors found (true HW vs virtual machine) :
  when comparing between:
  a "Real" Core 2 Duo T7100 and a "Virtual Machine" (Virtual Box on top of Windows 7 with Intel(R) Core™ i7-4800MQ)

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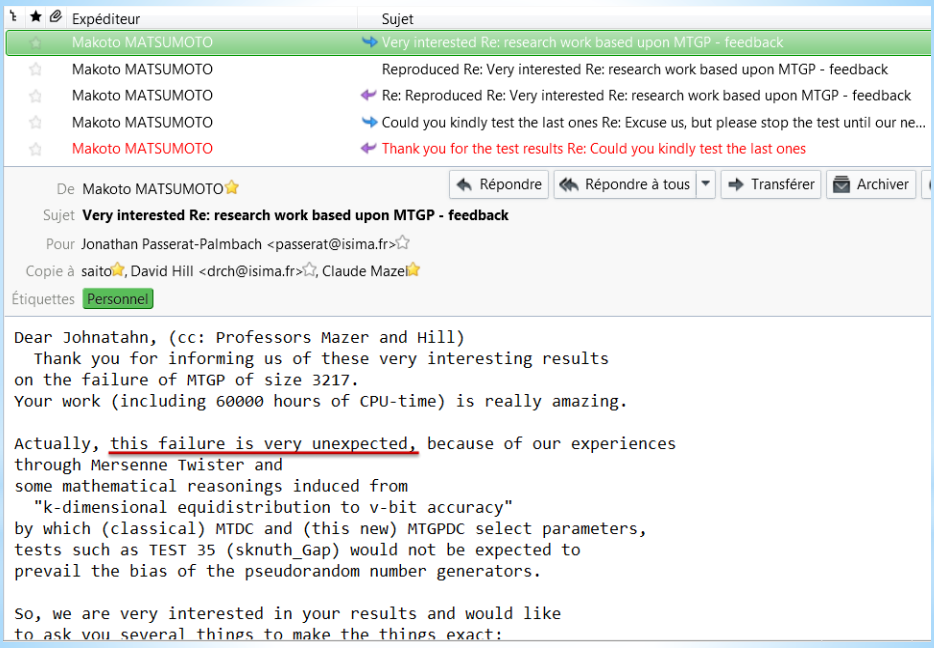
0.2675911	0.2675910
0.1784127	0.1784128

Table 7: Results for TinyMT_32 PRNG with open64-i386 on virtual machines of Ubuntu-13.04 and 14.04

Expected results CHECK32.OUT.TXT	Results obtained with Ubuntu 13 on Virtual Box	Results obtained of Ubuntu 14 on Virtual Box
0.6455914	0.6455913	0.6455913
0.9415597	0.9415598	0.9415598
0.9034473	0.9034472	0.9034472
0.9348063	0.9348064	0.9348064
0.7581965	0.7581964	0.7581964

- **Will this impact Docker for Windows since it works on top of virtual Box ?**



	Expéditeur	Sujet
☆	Makoto MATSUMOTO	Very interested Re: research work based upon MTGP - feedback
☆	Makoto MATSUMOTO	Reproduced Re: Very interested Re: research work based upon MTGP - feedback
☆	Makoto MATSUMOTO	Re: Reproduced Re: Very interested Re: research work based upon MTGP - feedback
☆	Makoto MATSUMOTO	Could you kindly test the last ones Re: Excuse us, but please stop the test until our ne...
☆	Makoto MATSUMOTO	Thank you for the test results Re: Could you kindly test the last ones

De Makoto MATSUMOTO

Répondre | Répondre à tous | Transférer | Archiver

Sujet **Very interested Re: research work based upon MTGP - feedback**

Pour Jonathan Passerat-Palmbach <passerat@isima.fr>

Copie à saito, David Hill <drch@isima.fr>, Claude Mazel

Étiquettes Personnel

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Dear Johnatahn, (cc: Professors Mazer and Hill)
  Thank you for informing us of these very interesting results
on the failure of MTGP of size 3217.
Your work (including 60000 hours of CPU-time) is really amazing.

Actually, this failure is very unexpected, because of our experiences
through Mersenne Twister and
some mathematical reasonings induced from
  "k-dimensional equidistribution to v-bit accuracy"
by which (classical) MTDC and (this new) MTGPDC select parameters,
tests such as TEST 35 (sknuth_Gap) would not be expected to
prevail the bias of the pseudorandom number generators.

So, we are very interested in your results and would like
to ask you several things to make the things exact:
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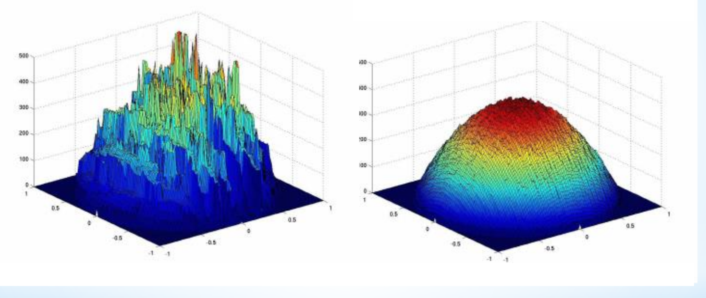
Remember: let's « see » the potential impact of the generator quality…



Two results of the same simulation (sequential) – PDE Harmonic solution computed with Brownian movements.
On the left the image is obtained with Linux rand (which is already far better than the old std UNIX rand on 15bits)
On the right – same simulation with Mastumoto Mersenne Twister (1997 version) – right solution elipsoid with a circular section.

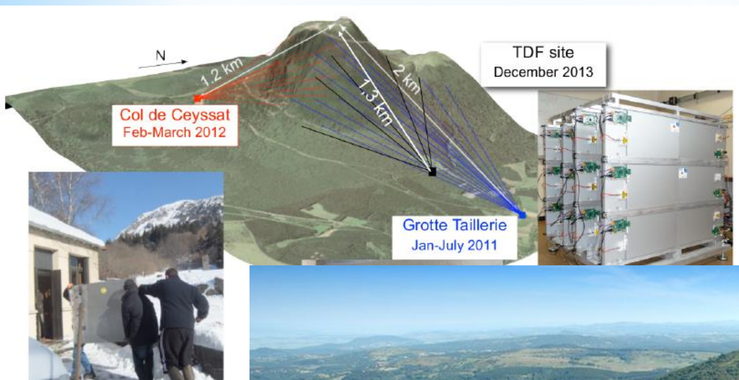
Some top PRNGs (Pseudo Random Number Generators)

Only Green PRNG are recommended:

- LCG (Linear Congruential Generator) - $x_i = (a^*x_{i-1} + c) \bmod m$
  forget them for Scientific Computing see [L'Ecuyer 2010]
- LCGPM (Linear Congruential Generator with Prime Modulus – could be Mersenne or Sophie Germain primes)
- MRG (Multiple Recursive Generator)
  $x_i = (a_1^*x_{i-1} + a_2^*x_{i-2} + \ldots + a_k^*x_{i-k} + c) \bmod m$ – with k>1
- (Ex: MRG32k3a & MRG32kp – by L'Ecuyer and Panneton)
- LFG (Lagged Fibonacci Generator)
  $x_i = x_{i-p} \square x_{i-q}$
- MLFG (Multiple Lagged Fibonacci Generator) – Non linear by Michael Mascagni MLFG 6331_64
- L & GFSR (Generalised FeedBack Shift Register…) Mod 2
- Mersenne Twisters – by Matsumoto, Nishimura, Saito (MT, SFMT, MTGP, TinyMT) – **WELLs** Matsumoto, L'Ecuyer, Panneton

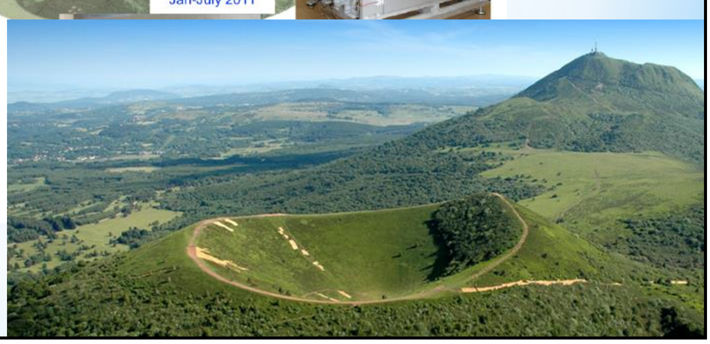
See [Hill et al 2013] for advices including hardware accelerators

Reproducible HPC Application Muonic Tomography - billions of threads…

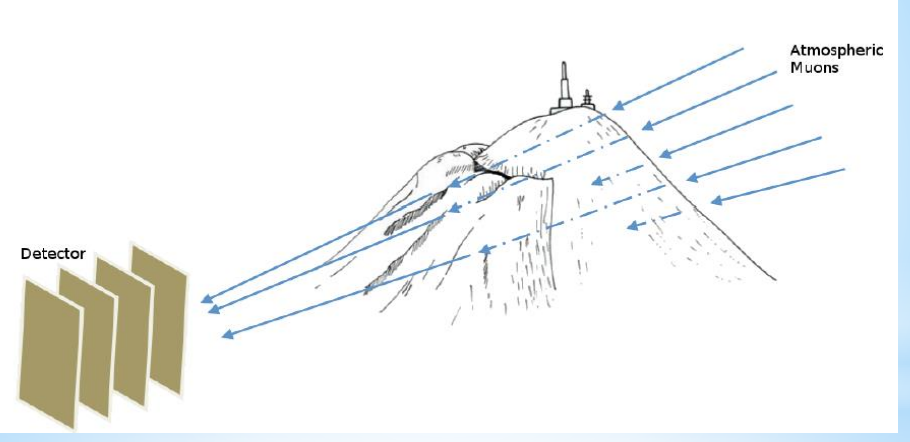


Puy de Dôme Volcano France

Places of atmospheric Muons sensors

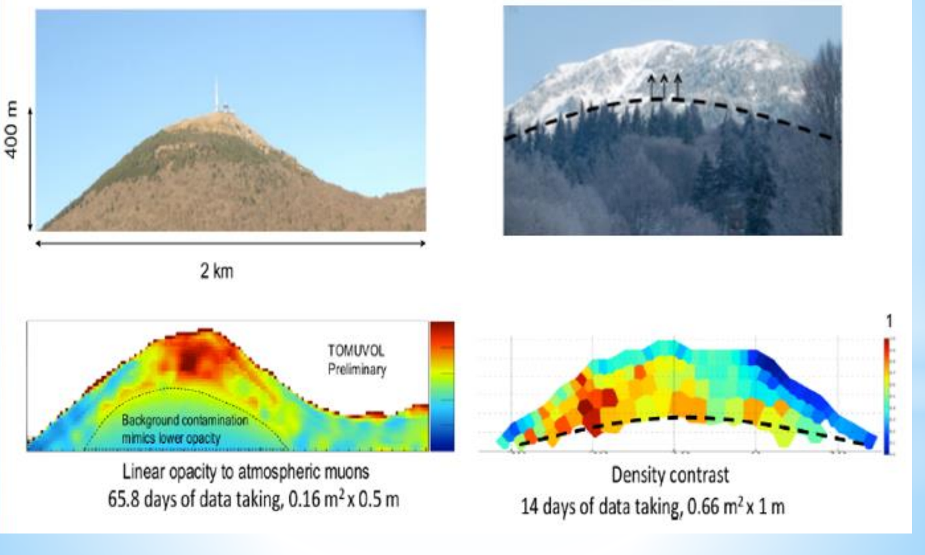


Principle of muonic tomography



Principle: atmospheric muons will go through matter. Depending on their energy and of the matter they traverse it is possible to reconstruct the 3D inner image of a large edifice with multiple sensors (figure by Samuel Béné)

2D Tomographic rendering



Linear opacity to atmospheric muons
65.8 days of data taking, 0.16 m² x 0.5 m

Density contrast
14 days of data taking, 0.66 m² x 1 m

Optimization for a single « hybrid » node (Intel E52650 & Xeon Phi 7120P)

Parallel stochastic simulation of muonic tomography

- Parallel programming model using p-threads
- On stochastic object for each Muon
- Multiple streams using MRG32k3a[1]
- A billion threads handled by a single node
- Compiling flags set to maximum reproducibility

Table 3: Performance of a billion event simulation when parallelized on 1 Phi, 1 CPU, 2 CPUs

	Intel Xeon Phi 7120P	Intel Xeon E5-2650v2	2x Intel Xeon E5-2650v2
Time	48 h 49 min	36 h 32 min	18 h 17 min
Speedup	1	1.34	2.67

(1) P. L'Ecuyer, R. Simard, E. J. Chen, and W. D. Kelton, ``An Objected-Oriented Random-Number Package with Many Long Streams and Substreams", Operations Research, Vol. 50, no. 6 (2002), pp. 1073-1075.

Bit for bit reproducibility

Do not expect bit for bit reproducibility when working on Intel Phi vs. regular Intel processors[1].

- We observed bit for bit reproducibility in single precision but not in double precision (and with the expected compiler flags)
- The relative difference between processors (E5 vs Phi) in double precision were analyzed and are shown below:

Table 1: Relative CPU-Phi differences between the results and number of altered bits

Difference ↓ \ Result →	Position X	Position Z	Direction X	Direction Y	Direction Z
0 bit: bit for bit reproducibility	4922	4934	4896	4975	4913
1 bit: 1.11E-16 ≤ Δ < 2.22E-16	25	21	14	5	18
2 bits: 2.22E-16 ≤ Δ < 4.44E-16	21	18	52	4	31
3 bits: 4.44E-16 ≤ Δ < 8.88E-16	15	12	23	6	12
4 bits: 8.88E-16 ≤ Δ < 1.78E-15	10	7	5	4	10
≥ 5 bits: 1.78E-15 ≤ Δ < 2.25E-11	7	8	10	6	16

(1) Run-to-Run Reproducibility of Floating-Point Calculations for Applications on Intel® Xeon Phi™ Coprocessors (and Intel® Xeon® Processors) – by Martin Cordel
https://software.intel.com/en-us/articles/run-to-run-reproducibility-of-floating-point-calculations-for-applications-on-intel-xeon

Relative difference (Phi vs E5)

The results on the two architectures are of the same order,

Both of them have the same sign and the same exponent (even if some exceptions would be theoretically possible, they would be very rare).

The only bits that can differ between these results are the least significant bits of the significand.

For a given exponent e, and a result $r1 = m \times 2e$, the closest value greater than r1 is $r2 = (m + \varepsilon d) \times 2e$, where εd is the value of the least significant bit of the significand: $\varepsilon d = 2^{-52} \approx 2.22\ 10^{-16}$.

Intel Compiler flags:

- ✓ "`-fp-model precise -fp-model source -fimf-precision=high -no-fma`" for the compilation on the Xeon Phi
- ✓ "`-fp-model precise -fp-model source -fimf-precision=high`" for the compilation on the Xeon CPU.

Conclusion

- **Repetability achieved on identical execution plaforms**
- **Numerical differences are reduced between classical Xeon and Intel Xeon Phi (different HW - x86 vs k1om)**
- **Numerical Reproducibility is possible for Parallel Stochastic applications with independent computing on homogeneous nodes.**
- **This approach can be used for low reliability supercomputers (with current MTTF below 1 day)**
- Key elements of a method have been presented to give numerically reproducible results for parallel stochastic simulations comparable with a sequential implementation (before large scaling on future Exascale systems)
- Numerical replication is very important for scientists in many sensitive areas, finance, nuclear safety, medicine…

Perspectives

- **Simulation of parallel independent processes can be now considered as "easy",** but simulating time-dependent entities or interacting entities, with numerical reproducibility across interactions and cross various heterogeneous communicating nodes will be tough.
- Software simulation of co-routines within the simulation application and synchronous communications can be required in addition to the assignment of a different random streams to each stochastic object.
- Numerical replication is very important for scientists in many sensitive areas, finance, nuclear safety, medicine, national security.
- Get prepared with Fault Injection frameworks like (SEFI – Los Alamos National Library, USA) 23

Définitions:

Accuracy :
nombre de chiffres corrects sur un calcul

Precision :
nombres de bits utilisés pour le calcul

Can have the same errors : but with reproducibility