Parallel Stochastic Simulations “Reproducibility & Ethical Research”

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(Credit : Pierre Schweitzer – Claude Mazel and Dao Van Toan)
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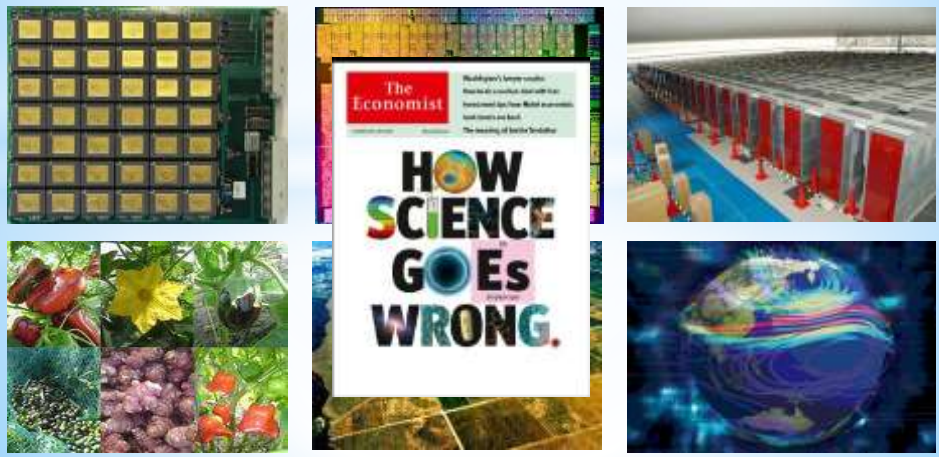
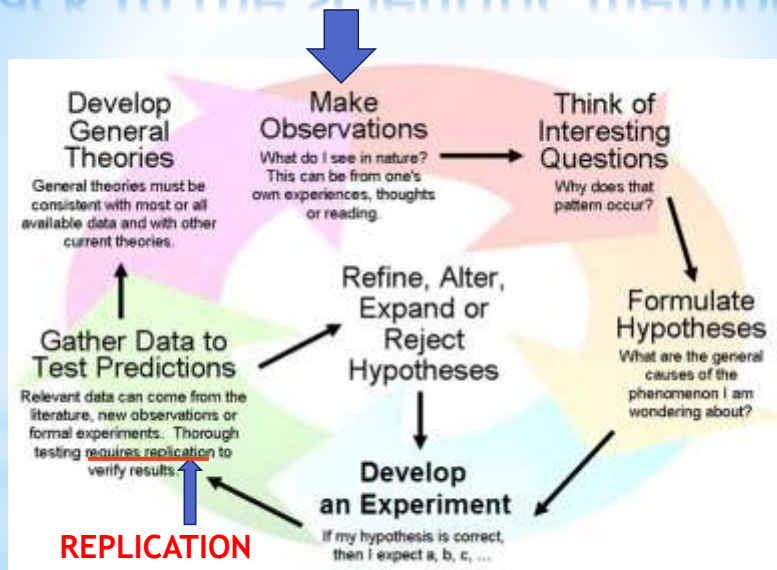


Back to the scientific method



https://i0.wp.com/peegel.info/wp-content/uploads/2017/10/scientific_method.png

Criterions of the scientific method

The major criteria of the scientific method are **intangible principles** :

- **Refutability :** a scientific affirmation is said to be rebuttable if it is possible to record an observation or conduct an experiment which, if it were positive, would contradict this statement.
- **Non-contradiction :** is the law that prohibits affirming and denying the same term or proposition
- **Reproducibility** : Science works by drawing "laws" or "principles" from **reproducible observations** whose main property is to be true as long as no observation has proved otherwise.

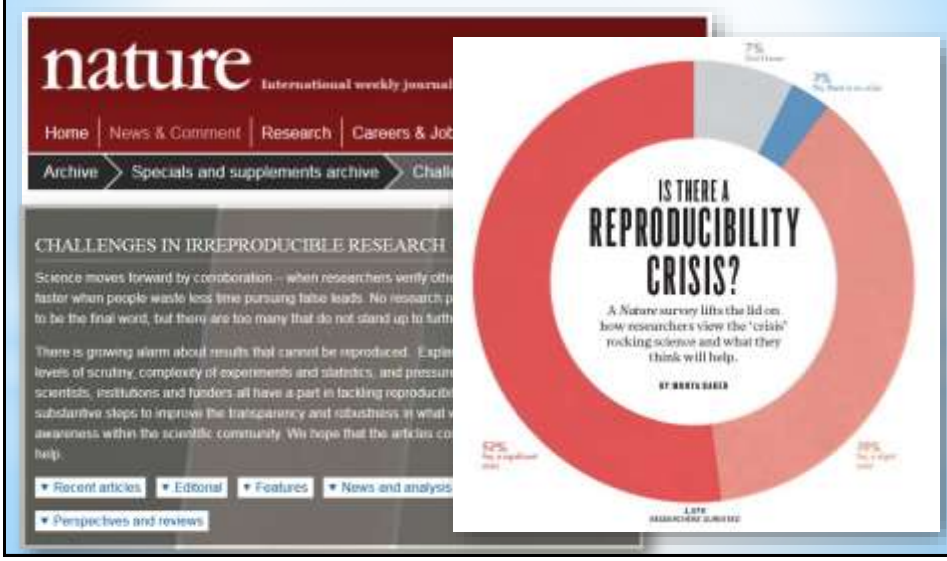
Reproducibility for beginners

Research is **repeatable** if we can re-run the researchers' experiment using the same method in the same environment and obtain the same results.
Unfortunately, it is not often the case…

Reproducibility…

- Many of us know the important work of Karl Popper (philosopher of sciences) in modeling and simulation. Karl Popper is generally regarded as one of the greatest philosophers of Science of the 20th century.
- The criterion of **reproducibility** is one of the conditions on which Popper distinguishes between the scientific or **pseudo-scientific** character of a study.
- Scientific conclusions **can only be drawn from a well observed and described "event", which has appeared several times**, observed by different people and/or studies.
- This criterion **eliminates** random effects that distort the results as well as errors in judgment or manipulation by scientists.

A reproducibility crisis…



A problem existing in many domains

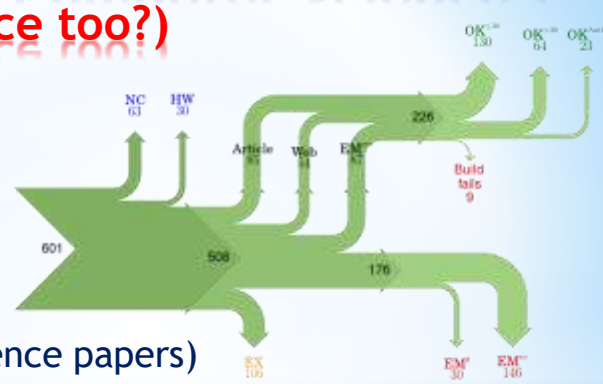
Reproducibility & corroboration

- Science moves forward by **corroboration** when researcher's verify each other's data.
- Science advances faster when people waste less time pursuing false leads.
- There is a growing alarms of results that have been published but **that cannot be reproduced**.

- In 2015 a study of top scientific research (REF) in UK showed that only 11% of medical studies where reproducible. (First page of "The Guardian")

What about Computer Science ?

(pseudo-science too?)



Repeatability:

A study of 601 'A' ranked papers (journal or conference papers) published by the distinguished ACM (Association for Computing Machinery) **showed that a only bit more than 30% of the results could be reproduced**

See : http://reproducibility.cs.arizona.edu/

How and why Science goes wrong ?!

1. Pressure to publish
2. Impact factor mania
3. Tainted resources
4. Bad maths
5. Sins of omission
6. Science is messy
7. Broken peer review
8. Some scientists don't share
9. Research never reported
10. Poor training -> sloppiness
11. Honest error
12. Fraud
13. Disorganisation & time pressures
14. Cost to prepare and curate materials
15. Inherently "unreplicable" (one-off data, specialist kit)

https://www.sciencenews.org/article/12-reasons-research-goes-wrong (adapted)

See : http://www.slideshare.net/carolegoble/open-sciencemcrgoble2015

1st Reason of failure : Pressure to Publish - impacting our scientific ethics…

The race for impact induces questionable practices. This is not fraud in the classical sense, but it's not good for trust in the published works.

- We slice our work to get more papers where only one would have been enough.
- We exaggerate the importance of a study to make it more attractive.
- We cite top scientists to attract their benevolence.
- We increase self-citation to "go up" in the rankings.
- And many other practices to cope with this pressure…

The traditional ["publish or perish"] has become [impact or perish "]

In 2016 Mario Biagioli who, in 2016 has led a symposium on the links between the development of metrics and scientific misconduct.

The system is he pushed to crime as commented by Laments Catherine Jessus, head of Life Sciences at the French National Research Center (CNRS).

A major obstacle for many scientists…

- **Confidence in peers…**
- Without data and code sharing : exit reproducibility…

Another obstacle : Publication interests of most Journals…

"Unfortunately we receive many more papers than we can publish or indeed review and must make difficult decisions on the basis of novelty and general interest as well as technical correctness."

"Reject without review…"

It happens increasingly often, especially if you send work to journals with high impact factors.

http://deevybee.blogspot.fr/2012/01/novelty-interest-and-replicability.html

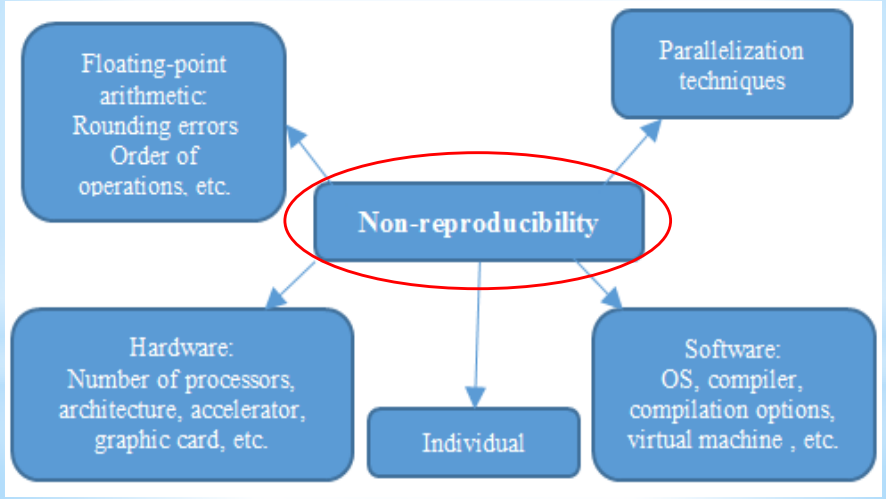
Reproducibility ? (some defn.)

- 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 (COMPUTER ORIENTED)
  - ✓ "*Reproducibility, i.e. **getting bitwise identical results from run to run***"
- In Revol and Théveny 2013 (COMPUTER ORIENTED TOO)
  - ✓ "*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



Now SC too is concerned – Top journals take care, don't miss the train…

Ex: Zoom in technical some reasons like « Out of Order Execution » of floating point instructions

- Out-of-order execution is also known as **dynamic execution**. Most **modern high-performance microprocessors** optimize the execution of instructions based on the availability of input data to avoid delays.
- **The original order of instructions in a program is not respected !**
- The micro-processor avoids having parts of its internal computing units being idle by processing the next instructions which are able to run immediately and “independently”.
- It is the equivalent of the software dynamic recompilation (or just-in-time compilation) which enables improving instruction scheduling.
- Remember: **floating point arithmetic is not associative** (for + & *)
  ex: a+(b+c) != (a+b)+c.

$$(10^{-3}+1)-1 \sim 0$$
$$10^{-3}+(1-1)=10^{-3}$$

```
>>> (pow(10,-3)+1)-1
0.000999999999999988899
>>> pow(10,-3)+(1-1)
0.001
>>>
```

Recent microprocessor design errors and dangerous miss-behaviors

[WARNING] Intel Skylake/Kaby Lake processors: broken hyper ...
https://lists.debian.org/debian-devel/2017/06/msg00308.html ▾ Traduire cette page
25 juin 2017 - TL;DR: unfixed **Skylake** and **Kaby Lake** processors could, in some situations, dangerously misbehave when **hyper-threading** is enabled. Disable **hyper-threading** immediately in BIOS/UEFI to work around the **problem**. Read this advisory for instructions about an Intel-provided fix. SO, WHAT IS THIS ALL ...

Intel répond au bug de l'Hyperthreading Skylake et Kaby Lake sous ...
Users of systems with Intel Skylake processors may have two choices:

1. If your processor model (listed in /proc/cpuinfo) is 78 or 94, and the stepping is 3, install the non-free "intel-microcode" package with base version 3.20170511.1, and reboot the system. THIS IS THE RECOMMENDED SOLUTION FOR THESE SYSTEMS, AS IT FIXES OTHER PROCESSOR ISSUES AS WELL.

Skylake and Kaby Lake CPUs have broken hyper-threading - Fudzilla
https://www.fudzilla.com/.../43964-skylake-and-kaby-lake-cpus-ha... ▾ Traduire cette page
26 juin 2017 - During April and May, Intel started updating processor documentation with a new errata note and it turned out that the reason was that **Skylake** and **Kaby Lake** silicon has a microcode bug it did not want any one to find out about. The errata is described in detail on the Debian mailing list, and affects **Skylake** ...

Another example with software : if you use Java look at this paper and presentation…

How Java's Floating-Point Hurts Everyone Everywhere

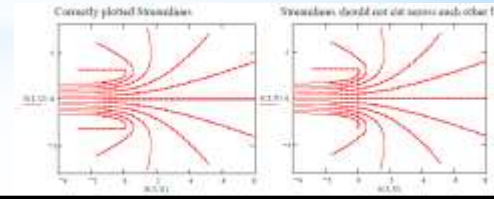
by
Prof. W. Kahan and Joseph D. Darcy
Elect. Eng. & Computer Science
Univ. of Calif. @ Berkeley

This document: http://www.cs.berkeley.edu/~wkahan/JAVAhurt.pdf or
http://www.cs.berkeley.edu/~darcy/JAVAhurt.pdf

Prof. Kahan – is THE leader for IEEE 754 Floating-Point standard.

Numerically non-expert programmers are legion

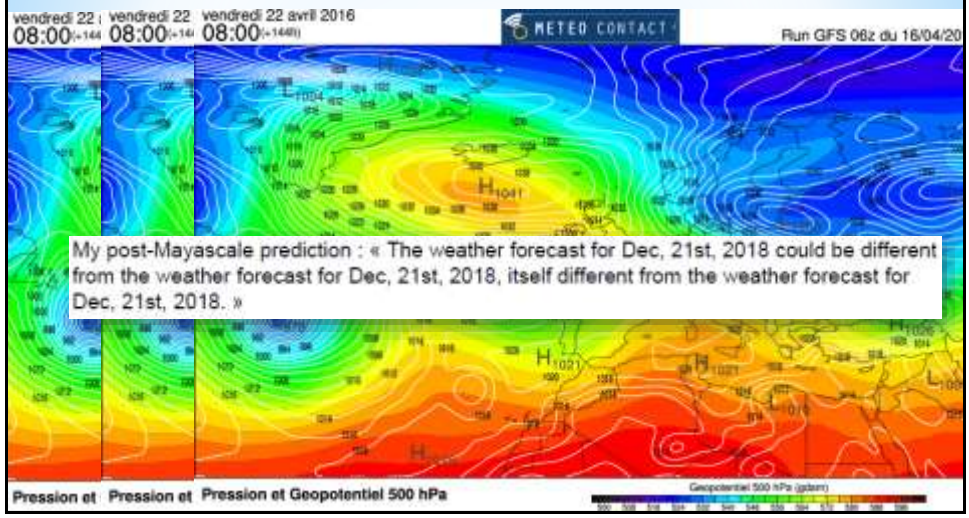
Error-analysis can be very unobvious



Competent error-analysts are extremely rare…

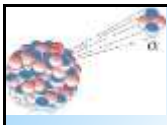
Run to run repeatability errors found Toulouse CERFACS & IBM

See the work of Francois Thomas – Optimisation of weather applications on Power and x86 architectures - Oct, 3rd 2012



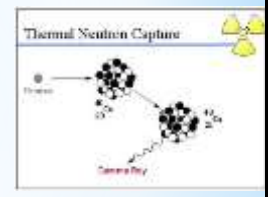
Exascale Computing soon available
(reproducibility pbs. at huge scales…)

- The goal of Exascale computing is to multiply by **10x** the performance of the fastest machine on operation.
- We can anticipate that Exascale systems will have around 10^9 computing cores.
- This also means that at the same time each standard nodes will be able to deliver tenths of teraflops.
- This will help to generate much faster, more precise and more complex simulations, higher quality medical imaging will yield faster and personalized medicine with smarter medical diagnostic and treatment.
- **Parallel Stochastic simulations will become more and more useful at this scale, particularly because they can be "fault" tolerant.**



Reliability & HPC…
…Silent & Soft errors…

1. Change the system state (external forces)
   - ✓ Alpha particles
   - ✓ Cosmic rays (High Energy Particles from space)
   - ✓ Thermal neutrons
   - ✓ Variation in voltage, temperature, etc.



2. They are at the origin of ECC…
   1. To avoids bits flips in memory cells
   2. There is also a rising of soft errors in arithmetic units !!!
   3. The more we size down the more this problem increases.
   4. Chip manufacturers spend money and silicon space to avoid this kind of errors
3. Soft errors are difficult to detect and reproduce – (using spare time of Titan - Still ranked 5 in current Top 500) ?

Reproducibility…

Parallel Stochastic Simulations – can be resilient to soft errors

- Easier when your model fits 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, Quantum ?…)

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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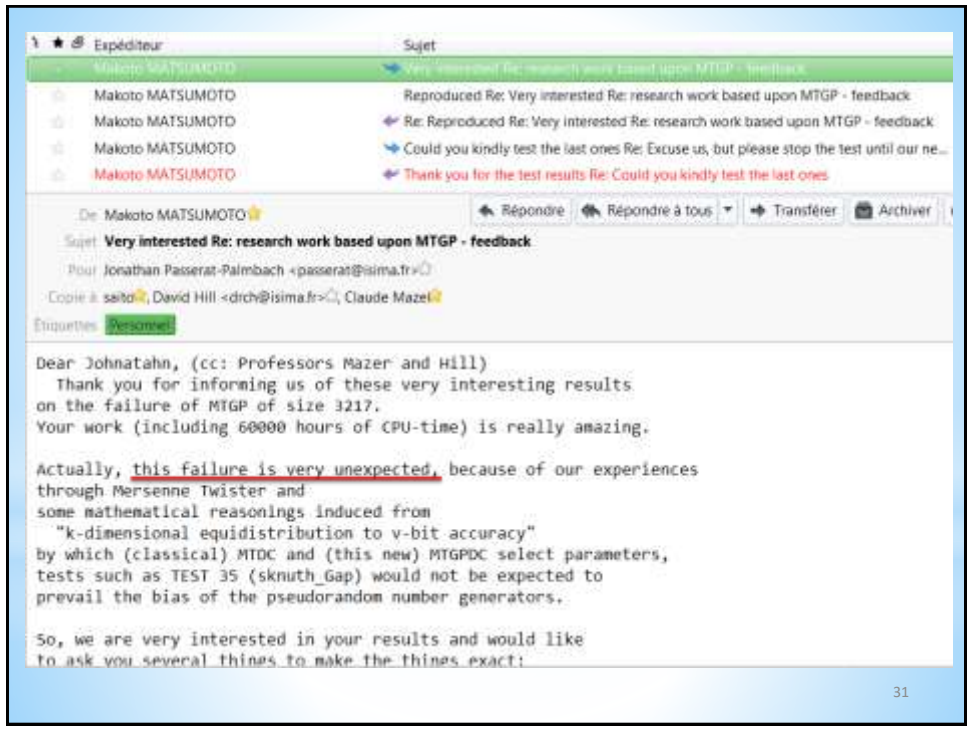
0.4688578	0.4688579
0.2675911	0.2675910
0.1784127	0.1784128

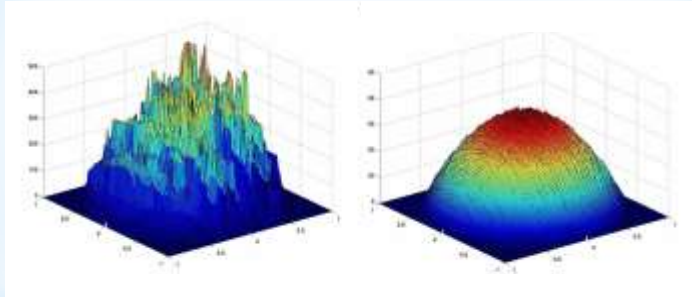
Table 7: Results for TinyMT_32 PRNG with open64-i386 on virtual machines of Ubuntu-13.04 and 14.04

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 ?**



* 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.

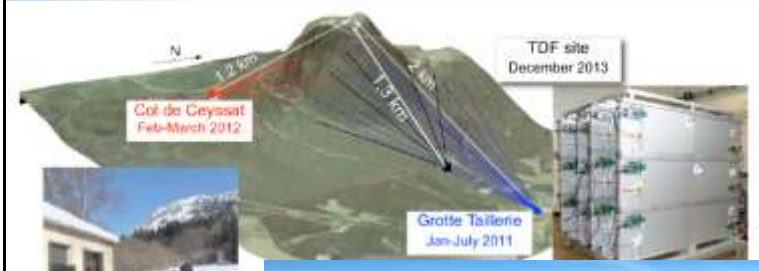
Some top PRNGs (Pseudo Random Number Generators)

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

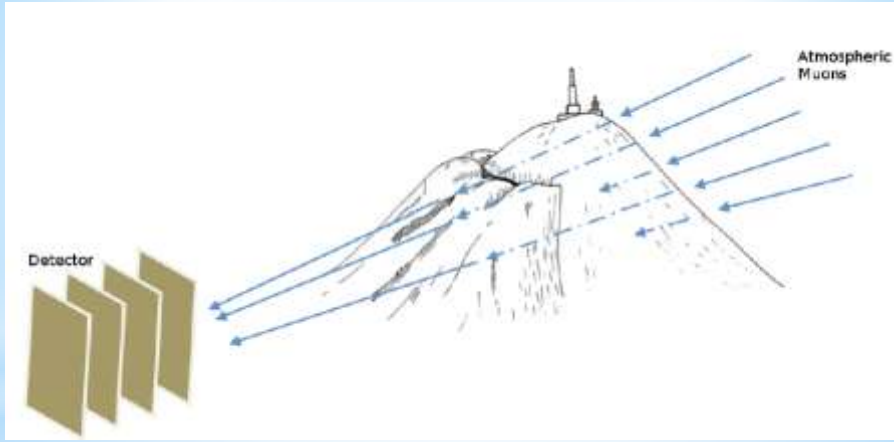
Reproducible HPC Application
Muonic Tomography - billions of threads…



Puy de Dôme
Volcano
France

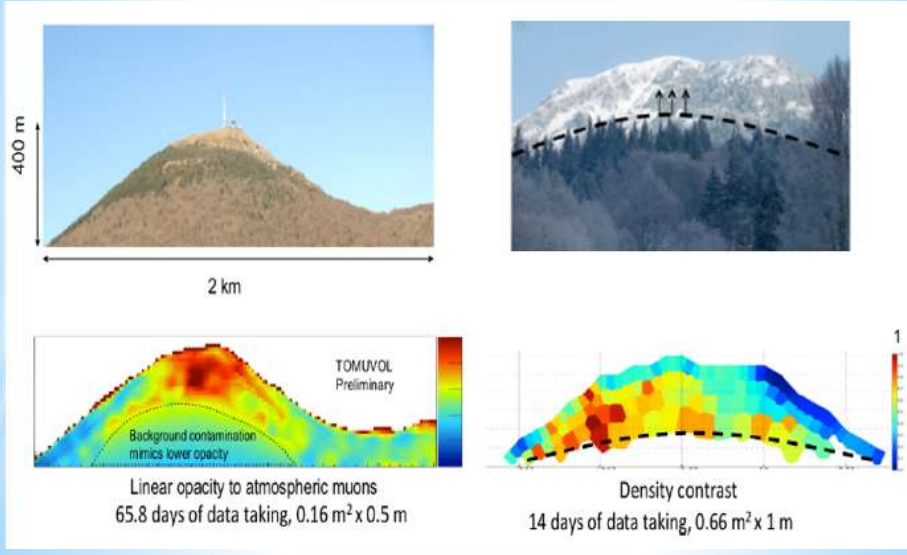
Places of atmospheric Muons sensors

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: $1.11E\text{-}16 \leq \Delta < 2.22E\text{-}16$	25	21	14	5	18
2 bits: $2.22E\text{-}16 \leq \Delta < 4.44E\text{-}16$	21	18	52	4	31
3 bits: $4.44E\text{-}16 \leq \Delta < 8.88E\text{-}16$	15	12	23	6	12
4 bits: $8.88E\text{-}16 \leq \Delta < 1.78E\text{-}15$	10	7	5	4	10
$\geq$ 5 bits: $1.78E\text{-}15 \leq \Delta < 2.25E\text{-}11$	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 × 2e, the closest value greater than r1 is r2 = (m + εd) × 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) 41

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