Simulation Parallèles Stochastiques "Reproductibles"?

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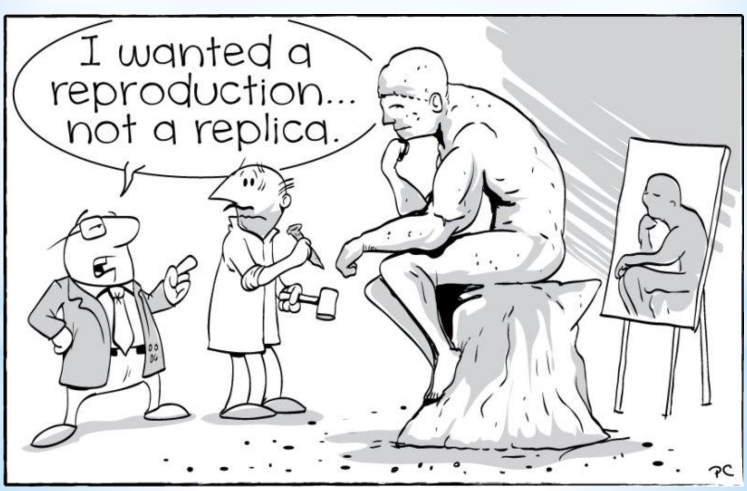
REPRODUCIBILITY BEGINNER's



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

Application Driven 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
1.15201260999473**6**	1.15201260999473**7**
1.36320183667365**0**	1.36320183667365**1**
1.21817093062946**3**	1.21817093062946**4**

Reproducing results - portability 3/4

- Errors found :
  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 :
  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)

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

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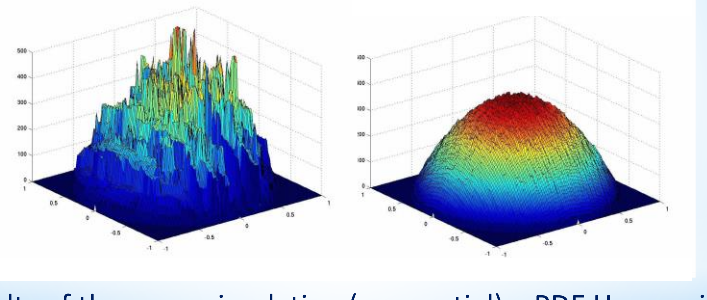
Table 7: Results for TinyMT_32 PRNG with open64-i386 on virtual machines of Ubuntu-13.04 and 14.04

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 ?**

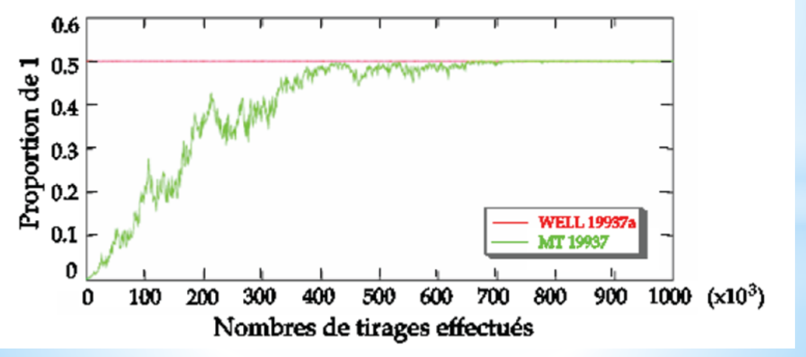
* Let's « see » the potential impact of the generator quality…



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.

* There is no perfect Generator… Ex: First Mersenne Twister : a known default…

Between 1997 and 2002 : very long recovery of **zero-excess initial state** for MT19237 (700 000 draws…)



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)
  $x_i = (a_1*x_{i-1} + a_2*x_{i-2} + \dots + a_k*x_{i-k} + c) \bmod m$ – 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

Quick survey of random streams parallelization

(1) Using the same generator

- The **Central Server** (CS) technique (avoid for flexible reproducibility)
- The **Leap Frog** (LF) technique. Means partitioning a sequence $\{x_i, i=0, 1, \ldots\}$ into 'n' sub-sequences, the j^{th} sub-sequence is $\{x_{kn+j-1}, k=0, 1, \ldots\}$ - like a deck of cards dealt to card players.
- The **Sequence Splitting** (SS) – or blocking or regular/fixed spacing technique. Means partitioning a sequence $\{x_i, i=0, 1, \ldots,\}$ into 'n' sub-sequences, the j^{th} sub-sequence is $\{x_{k+(j-1)m}, k=0, \ldots, m1\}$ where m is the length of each sub-sequence
  - Jump Ahead technique (can be used for both Leap Frog or Sequence splitting)
- The **Cycle Division** or **Jump ahead** approach. Analytical computing of the generator state in advance after a huge number of cycles (generations)
- The **Indexed Sequences** (IS) - or random spacing. Means that the generator is initialized with 'n' different seeds/statuses

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Quick survey of random streams parallelization

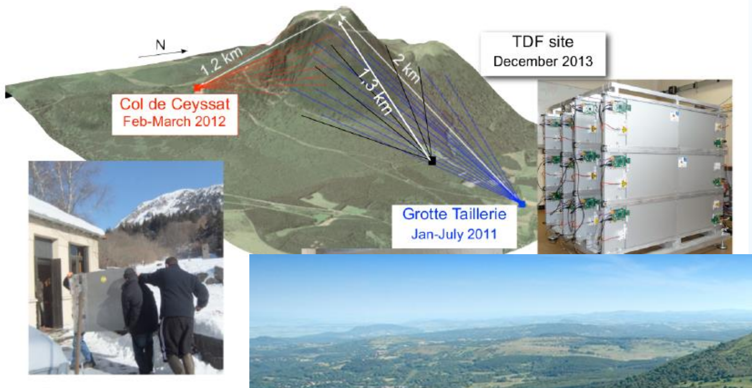
(2) Using different generators:

Parameterization:

The same type of generator is used with different parameters for each processor meaning that we produce different generators

- In the case of linear congruential generators (LCG), this can rapidly lead to poor results even when the parameters are very carefully checked. (Ex: Mascagni and Chi proposed that the modulus be Mersenne or Sophie Germain prime numbers)
- Explicit Inversive Congruential generator (EICG) with prime modulus has some very compelling properties for parallelizing via parameterizing.
- A recent paper describes an implementation of parallel random number sequences by varying a set of different parameters instead of splitting a single random sequence (Chi and Cao 2010).
- **In 2000 Matsumoto et al proposed a dynamic creation technique**

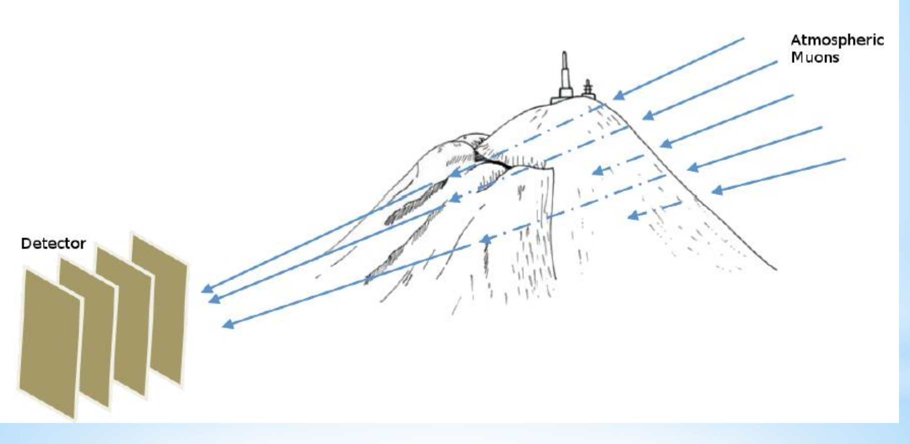
Reproducible HPC Application
Muonic Tomography - billions of threads…



Puy de Dôme
Volcano
France

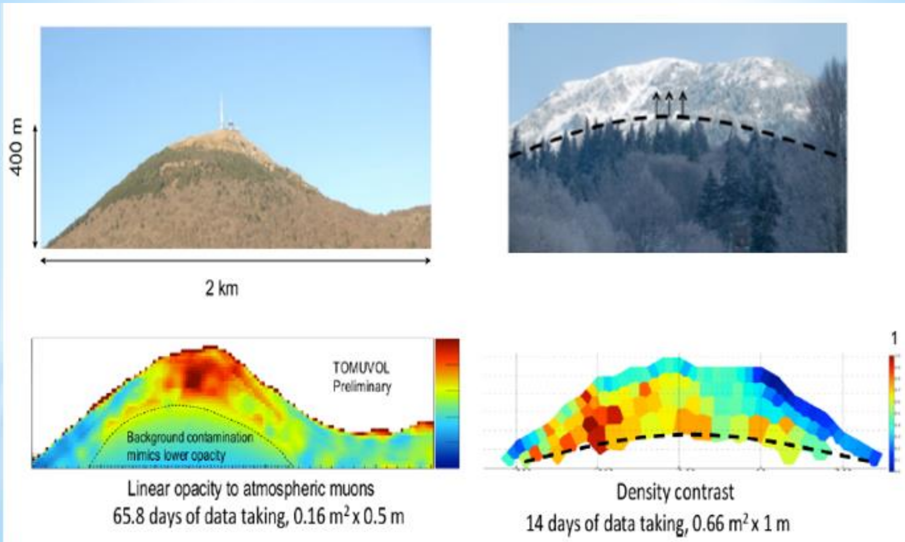
Places of atmospheric Muons sensors

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



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 × 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 reduced between classical Xeon and Intel Xeon Phi.
- 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 produced 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) 24

Spring 2016 Perspectives

Reproducibility Seminar for Computer Scientists in Auvergne with the input of Philosophers and Lawyers

- ✓ Reproducible Research
- ✓ Numerical Reproducibility
- ✓ Epistemology – how do we build knowledge
- ✓ Ethics and more…

Questions?