Numerical Algorithms for HPC

Random Number Generation

Introduction

- Random numbers are frequently used in many types of computer simulation
- Frequently as part of a sampling process:
  - Generate a representative sample of a large population by choosing members at random.
  - Monte-carlo integration is approximating an integral by sampling the function at random points.
  - Even when simulating a stochastic process (random walk/random events etc.) we are sampling the possible evolutions of the system.

What is Random anyway

- “Random” is actually a very difficult philosophical concept.
- However in most cases the real requirement is “unbiased sampling” which is more straightforward.

Distribution

- Random numbers are chosen from a probability distribution.
- For random integers each possible result *X* occurs with a probability P(*X*)
- For random real numbers *R* this becomes a probability density P(*R*)
  - Chance of the results occurring within a region is the integral of the probability density over that region.
  - Most generators are designed to generate a "uniform" distribution.
    - $P(R) = 1 \quad 0 <= R < 1$
    - $P(R) = 0$ elsewhere
    - Other distributions then generated from this

Resolution

- However computers use floating point numbers not true real numbers.
  - Only a finite set of possible values can be represented.
  - Any random “real” number must come from this set.
- Most techniques generate an even smaller sub-set of values e.g.
  - R = X/N where X is a random integer between 0 and N-1
  - 1/N is the resolution of that generator.
- Generated distribution is only an approximation to uniform.
  - May bias the results if you are not careful
  - Always worth understanding the resolution of your generator

Correlations

- True Random numbers are also un-correlated with each other.
- The probability of getting a particular set of random results should be the product of the probabilities of each result in isolation.

Hardware Random Number Generators

- You can build hardware random number generators.
  - These work by taking measurements of some random physical process
    - Thermal noise
    - Quantum processes.
  - Problems
    - Debugging is very hard as can never reproduce the same program run twice.
    - May still suffer from limited resolution
    - Often quite slow.
    - May not result in any visible improvement in quality of results.
  - More commonly used in cryptographic applications.

Pseudo Random Numbers

- Pseudo Random Numbers are a deterministic sequence of numbers generated by some algorithm that are used in-place of true random numbers.
- Aim is for the sequence to share enough of the statistical properties of true random numbers not to bias the results.
- PRNs are NOT random. It is always possible to come up with some test that demonstrates this.

PRNG Quality

- Quality of a PRNG sequence depends on the intended use.
  - Each use case only depends on *some* of the statistical properties of true random numbers.
  - Some generators may introduce problems for some calculations but not others.
- In practice, algorithms exist that can stand in for true random numbers for most common types of simulation.
- Unfortunately language default generators are often fairly poor.

Structure of a PRNG

- Logically PRNGs consist of:
  - An internal state S_i
  - An update transform $T\ S_i \rightarrow S_{i+1}$ that maps one state onto the next
  - An output transform $F\ S_i \rightarrow X_i$ that generates the next number in the PRNG sequence from the current state.
- Algorithms are rated on the statistical properties of the output sequence
  - Speed of execution and memory consumption are also important.
- Different algorithms may generate the same PRNG sequence via different state representations and transforms.

Seeding the Generator

- Also need some mechanism of initialising the starting state.
- Traditional algorithms only used a single word of state so many programs assume the generator is initialised using a single integer.
- If you don't set a starting seed you either:
    1. Get the same sequence every time you run the program.
    2. The generator seeds from the current time (makes debugging hard).
- If your program checkpoints remember to save RNG state so you can restart **exactly** where you left off.
    - Write tests to check this!

Period of a generator

- There are only a finite number of possible states.
- Eventually generator will return to its starting state.
- The update transform should generate a cyclic group $T^{period} = I$
- The size of this group is the *period* of the generator.
- It is also the number of valid states.

How state is stored

- In principle you could store the position in the sequence.
  - Update transform is just an increment $i \rightarrow i + 1$
  - All the randomness is in the output-transform.
  - Need very expensive output-transform to have good randomness properties.
- In practice use state representations that approximate random values and keep the output transform simple.
  - Even fairly simple (inexpensive) update transforms can have good randomness properties

PRNG Algorithms

- PRNG Algorithms are deceptively simple.
  - Usually made up from a few simple operations.
  - Typically bitwise operations or modular arithmetic.
- Very tempting to try and “Improve” on published algorithms
- DON’T DO THIS unless you really know what you are doing.
- Each new algorithm requires theoretical (Number theory) analysis to determine the period of the generator.
  - Many other statistical properties can also be derived theoretically.

Selecting Generators

- Most generators are selected based on the properties of small sets of consecutive numbers from the sequence.
  - $\{ X_i , X_{i+1} \}$ approximate a pair of random number.
- Non consecutive sets may appear less random.
  - E.g $\{ X_i , X_{i+1024} \}$
- Consecutive sets important for most applications (especially when used to generate non-uniform distributions) so this is a good heuristic for general purpose generators.
- For a specific application may be other correlations that are equally important.

- Selection uses a combination of theory and statistical tests.
- Statistical tests augment theory, not good enough by themselves.

Linear Congruential Generators

- $$S_{i+1} = (a\,S_i + c\,)\,mod\;\;M$$
- If a, c and M chosen correctly, has M possible states.
- If c = 0 then (M-1) possible states (S=0 always maps to itself).

Java.util.Random

- Optimised for speed not quality
  - a = 0x5DEECE66DL
  - C = 0xBL
  - M = 2^{48}
- Mod 2^{48} is a bit-mask so very fast.
- 47 bits of state in total.
  - However bit-n of the state has repeats with at most period 2^{n+1}
    - bit-0 period 2
    - bit-1 period 4
  - Only the high order bits repeat with any degree of randomness.
  - Class only exposes the top 32-bits to the user making it ok for quick and dirty use.

MRGs

- LCG are a special case of Multiply Recursive Generators
  - $S_n = a_1 S_{n-1} + \cdots + a_k S_{n-k} \ mod \ M$
  - Needs array of state variables.

- Some number theory ...

  - If $M = P^q$ with P prime then maximum period is $P^{q-1}(P^k - 1)$.
  - Special values of $\{ a_k \}$ generate full period if M is prime.

- Many other common generators are special cases of these.

Other Common generators

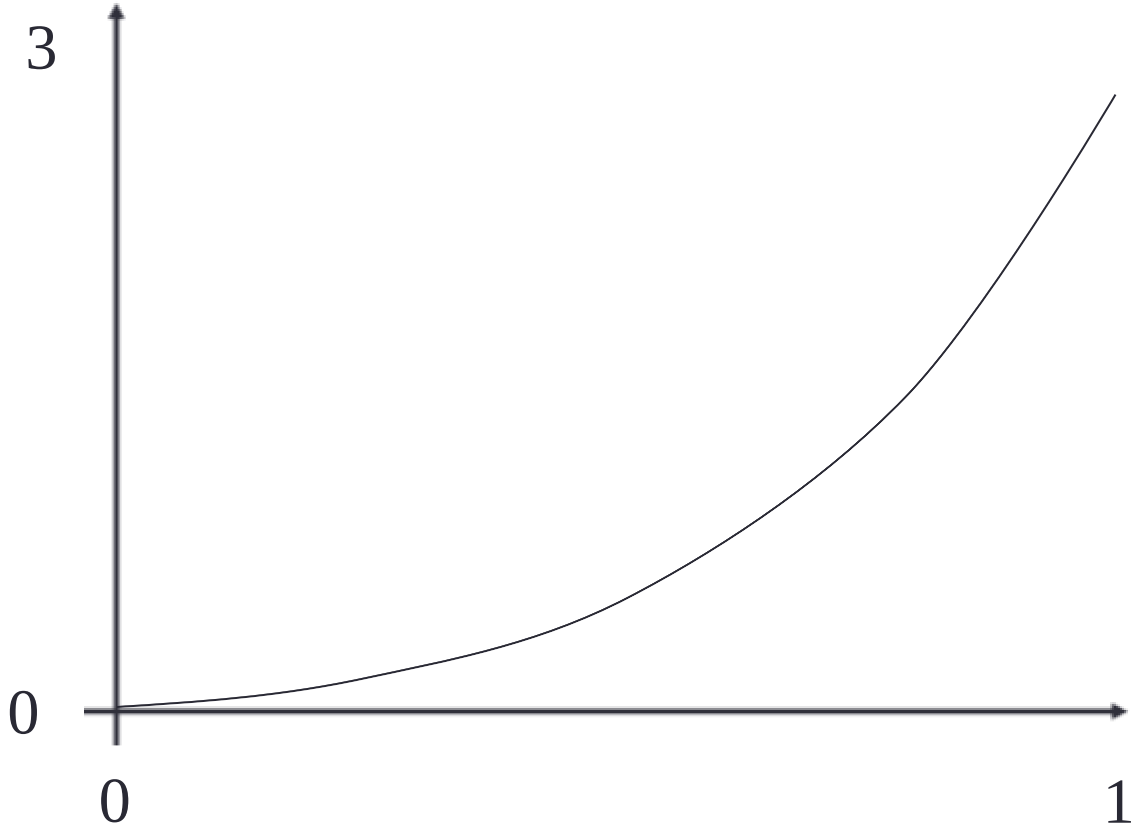
- LFSR
  - Linear Feedback Shift Register
  - M=2
- Lagged Fibonacci Generators
  - Only 2 Values of $\{ a_k \}$ non-zero so faster then the general case.
- Mersenne-Twister appears quite different but is equivalent to a MRG with M=2 and $(2^k - 1)$ a Mersenne prime.

Non uniform distributions

- Non-uniform distributions are constructed out of (multiple) normally distributed values.
- For any probability distribution $p(x)$
  - $\int_{min}^{max} p(x) = 1$
  - Selecting small areas under the curve uniformly is the same as selecting x with probability $p(x)$
  - Inverse transform sampling.
    - Divide area into thin strips of equal area and select strip at random.
  - Rejection sampling
    - Choose x,y points at random but reject points above curve i.e. $y > p(x)$

Simple example

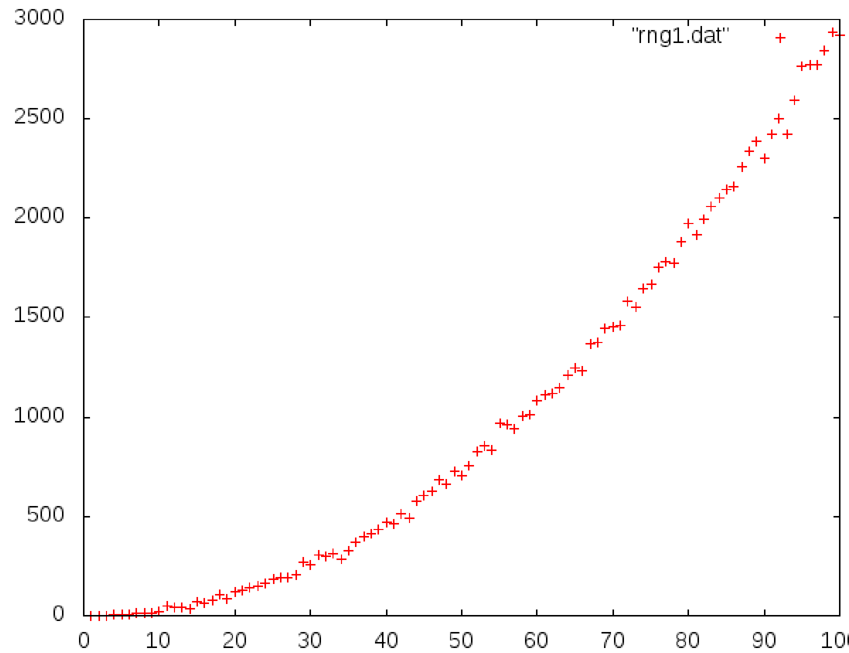
- $p(x) = 3x^2$



Inverse transform sampling

- Generally quite hard to do:
  - Generate uniform deviate U.
  - Return $x : \int_{min}^{x} p(y)dy = U$
- Only analytically solvable for certain distributions.
  - e.g for $p(x) = 3x^2$
  - $x = \sqrt[3]{U}$ (cube root of U)
  - 100,000 samples & 100 bins

```
call random_number(myrng)
myrng = myrng**(1.0/3.0)
```

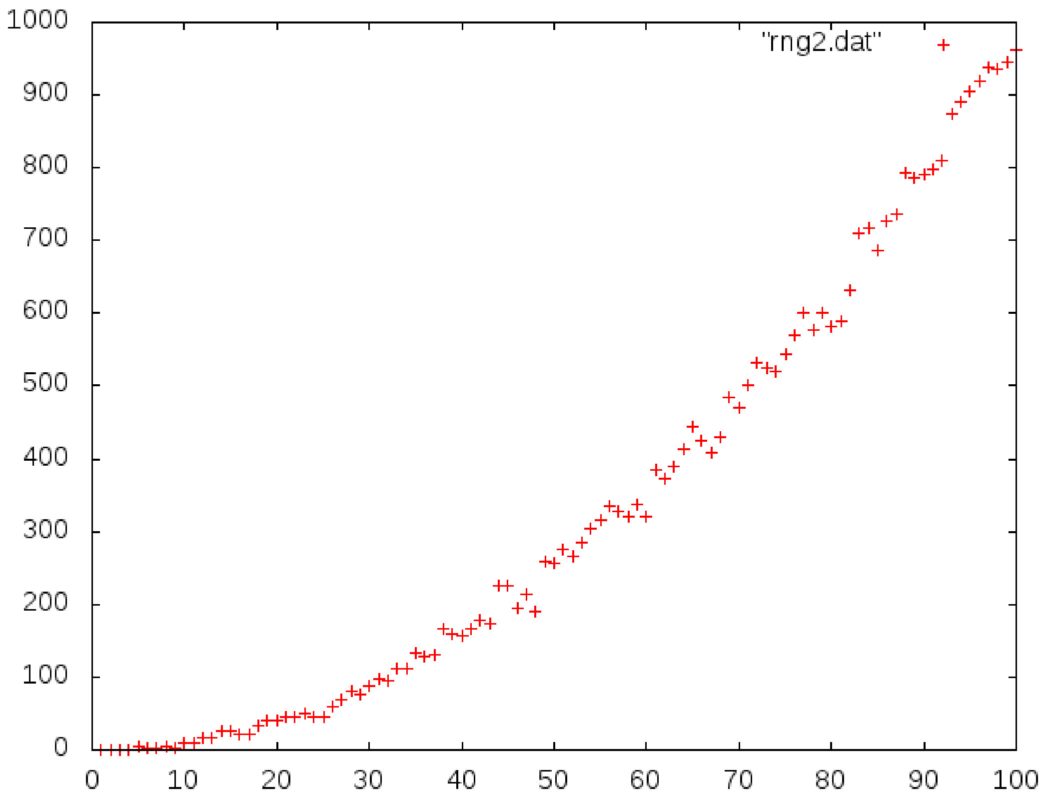


Rejection sampling

- Only need to be able to evaluate p(x).
  - Needs special handling for unbounded distributions.

- e.g for $p(x) = 3\,x^{2}$

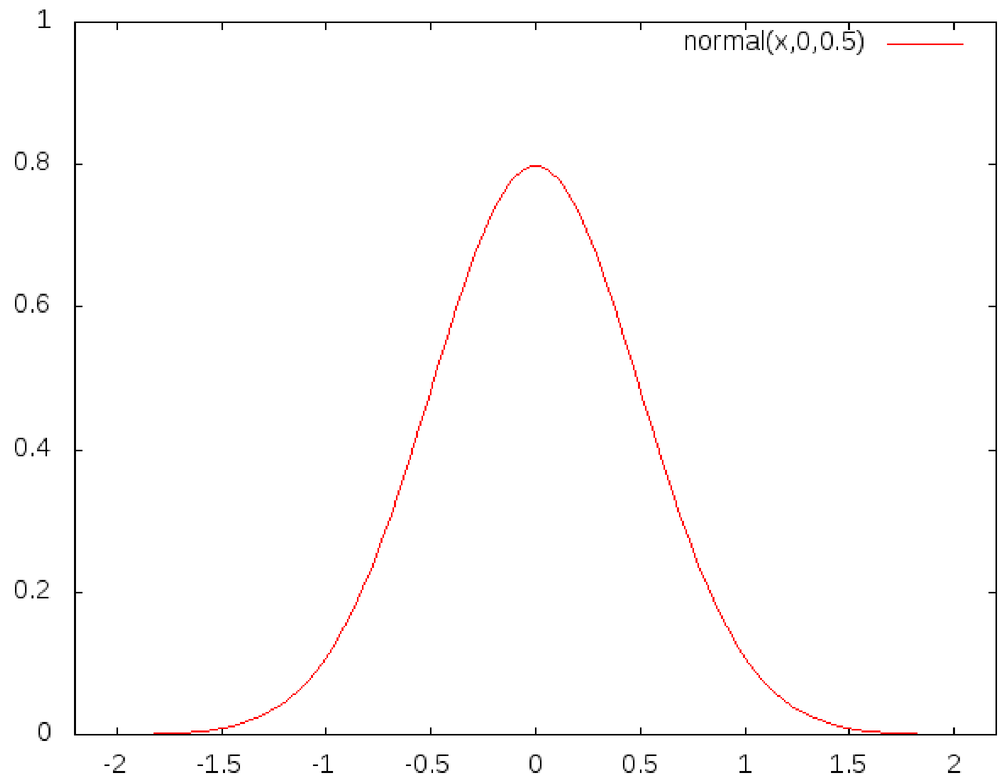
```
call random_number(myrng1)
call random_number(myrng2)
myrng2 = 3.0*myrng2
if (myrng2 < 3.0*myrng1**2)
  myrng = mynrng1
```



Generating Gaussians

- Most commonly required non-uniform distribution is the normal / gaussian distribution
  - $P(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-x^2}{2\sigma^2}}$

  -e.g for $\sigma = 0.5$



Box Muller

- Generates pairs of gaussians from pairs of uniform.
  - Generate 2 Uniform random numbers U,V from (0:1]
  - $X = \sqrt{-2\ln U}\,.\cos(2\pi\, V)$
  - Y= $\sqrt{-2\ln U}\,.\,sin(2\pi\, V)$
- Generally quite slow due to math library functions.
- With care an be vectorised so may be better algorithm for GPGPU.

Polar method

- Variation of box-muller that uses accept-reject step instead of trig functions.
  1. $a = 2\,U\ - 1$
  2. $b = 2\,V\ - 1$
  3. $s =\ a^2 + b^2$
  4. *If s > 1 goto (1)*
  5. $X = a\sqrt{\frac{-2\ln(s)}{s}}$
  6. Y$= b\sqrt{\frac{-2\ln(s)}{s}}$
- Usually faster overall but accept/reject inhibits vectorisation

Summary

- (Pseudo) random numbers are key to many algorithms
  - a number of high-quality algorithms exist
- Typically generate number in the range [0.0, 1.0)
  - includes 0.0 but excludes 1.0
  - e.g. generate “random” integer *i* in range 0 … *N*-1, return *i* / *N*
- Are often transformed to other distributions
  - analytically or using accept-reject stage
- Repeatability is a key requirement
  - necessary to test correctness of any computation
  - or interrupt and resume a long-running simulation