



993SM – Laboratory of Computational Physics II week March 6, 2023

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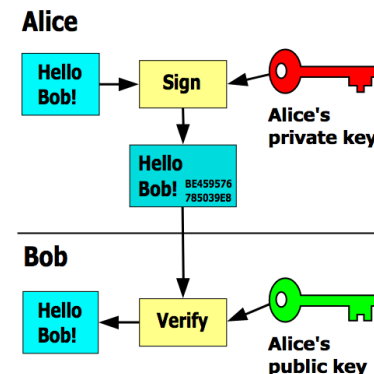
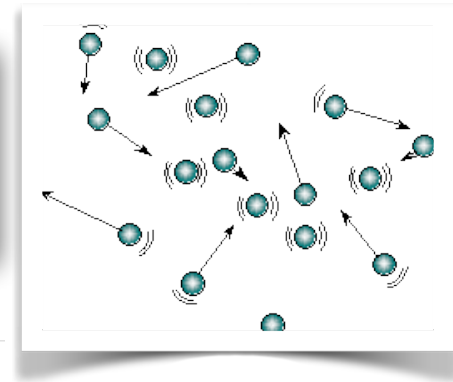
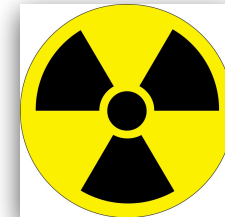
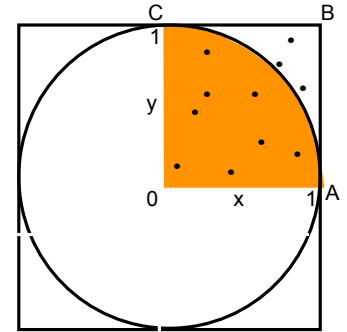
Random numbers and Monte Carlo(*) Techniques

(*) any procedure making use of random numbers

M. Peressi - UniTS - Laurea Magistrale in Physics
Laboratory of Computational Physics - II week

Random numbers: use

- in numerical analysis (to calculate integrals)
- to simulate and model complex or intrinsically random phenomena
- to generate data encryption keys
- ...



Random numbers: Characteristics and Generation

Random numbers

A sequence of random numbers is a set of numbers that have nothing to do with the other numbers in the sequence.

... but with a well defined statistical properties, e.g.:

In a uniform distribution of random numbers in the range $[0,1]$, every number has the same chance of turning up.

Note that 0.00001 is just as likely as 0.50000

True random numbers generation

- Use some chaotic systems, like numbered balls in a barrel (Lotto game)
- Use a process that is inherently random, such as:
 - radioactive decay
 - thermal noise
 - cosmic ray arrival
- Tables of a few million truly random numbers do exist, but this is not enough for most scientific applications

Pseudo random numbers generation with a computer

“pseudo” because they are necessarily generated with deterministic procedures
(the computer is a deterministic system!)

A sequence of computer generated random numbers
is not truly random, since each number is completely determined from the previous one.

But it may “appear” to be random.

(pseudo)Random numbers generation

These are sequences of numbers generated by computer algorithms, usually in a uniform distribution in the range $[0,1]$.

To be precise, the algorithms generate integers I_n between 0 and M , and return a real value.

$$x_n = I_n / M$$

the sequence may “appear” to be random

[Attention: in a Fortran code, write: $x_n = \text{float}(I_n)/M$!!!]

INTEGER

(pseudo)Random numbers generation

many different algorithms...

Two among the simplest (and oldest) algorithms:

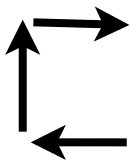
- von Neumann
- Linear Congruential Method

(pseudo)random numbers generation: example 1 - “Middle square” algorithm

(Von Neumann, 1946)

To generate a 10-digit integer sequence:

- take a first one
- square it
- consider the 10 central digits

loop 

eg. $5772156649^2 = 33317792380594909291$

so the next number is given by 

Also this sequence may “appear” to be random.

Limits of the algorithm:

depending on the initial choice, you can be trapped into short loops:

$6100^2 = 37210000$
 $2100^2 = 4410000$
 $4100^2 = 16810000$
 $8100^2 = 65610000$

(pseudo)random numbers generation: example II - “Linear congruential method (LCM)”

(Lehmer, 1948)

$$I_{n+1} = (a I_n + c) \bmod m$$

Starting value (seed) = I_0

a , c , and m are specially chosen

$a, c \geq 0$ and $m > I_0, a, c$

“ $A \bmod m$ ” is the
remainder
of the division of
 A by m

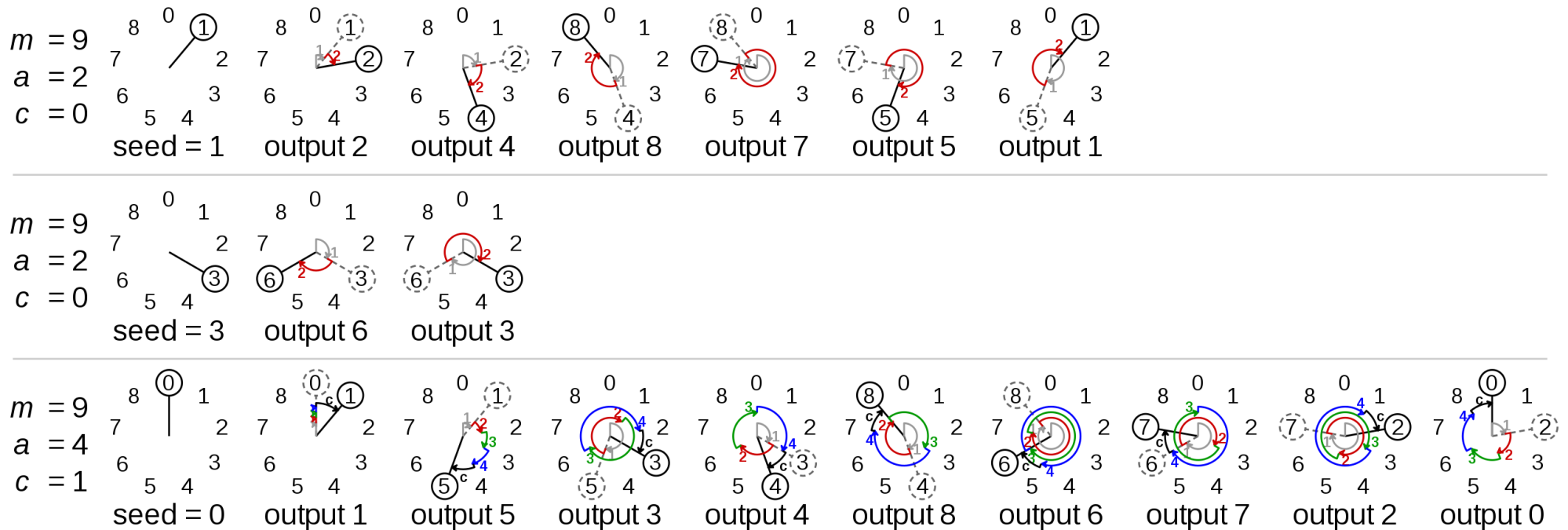
(pseudo)random numbers generation: example II - “Linear congruential method (LCM)”

$$I_{n+1} = (a I_n + c) \bmod m$$

QUESTIONS:

- in which interval are the pseudorandom numbers generated?
- Can we obtain all the numbers in such interval?
- Is the sequence periodic?
- Which is the period?
- Which is the maximum period?

(pseudo)random numbers generation: example II - “Linear congruential method (LCM)”



https://commons.wikimedia.org/wiki/File:Linear_congruential_generator_visualisation.svg

Limits of the algorithm:

- the “quality” of the sequence is very sensitive to the choice of the parameters
- even if $c \neq 0$

★ Choice of modulus, m

m should be as large as possible since the period can never be longer than m.

One usually chooses m to be near the largest integer that can be represented. On a 32 bit machine, that is $2^{31} \approx 2 \times 10^9$.

$$I_{n+1} = (a I_n + c) \bmod m$$

★ Choice of multiplier, a

It was proven by M. Greenberger in 1961 that the sequence will have period m, if and only if:

- i) c is relatively prime to m;
- ii) a-1 is a multiple of p, for every prime p dividing m;
- iii) a-1 is a multiple of 4, if m is a multiple of 4

More subtle limits, even of some smart algorithms...

A popular random number generator was distributed by IBM in the 1960's with the algorithm: <https://en.wikipedia.org/wiki/RANDU>

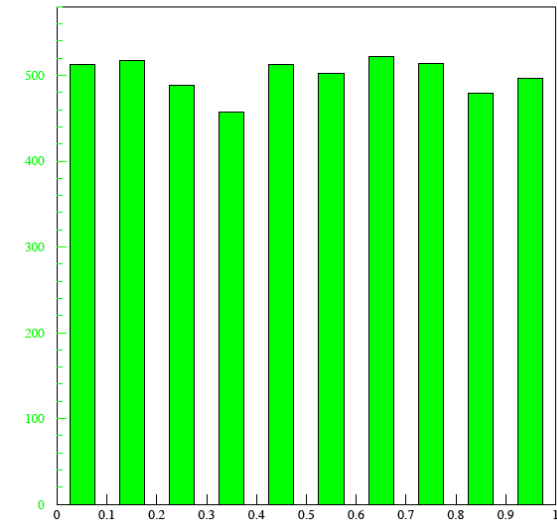
$$I_{n+1} = (65539 \times I_n) \bmod 2^{31}$$

$65539 = 2^{16} + 3$; initial seed I_0 : odd number

1D distribution Looks okay

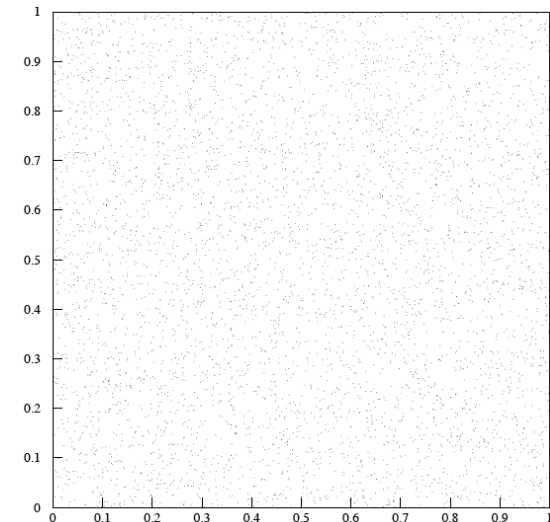
$\mathbf{x_i}, p(\mathbf{x_i})$

Results from Randu: 1D distribution



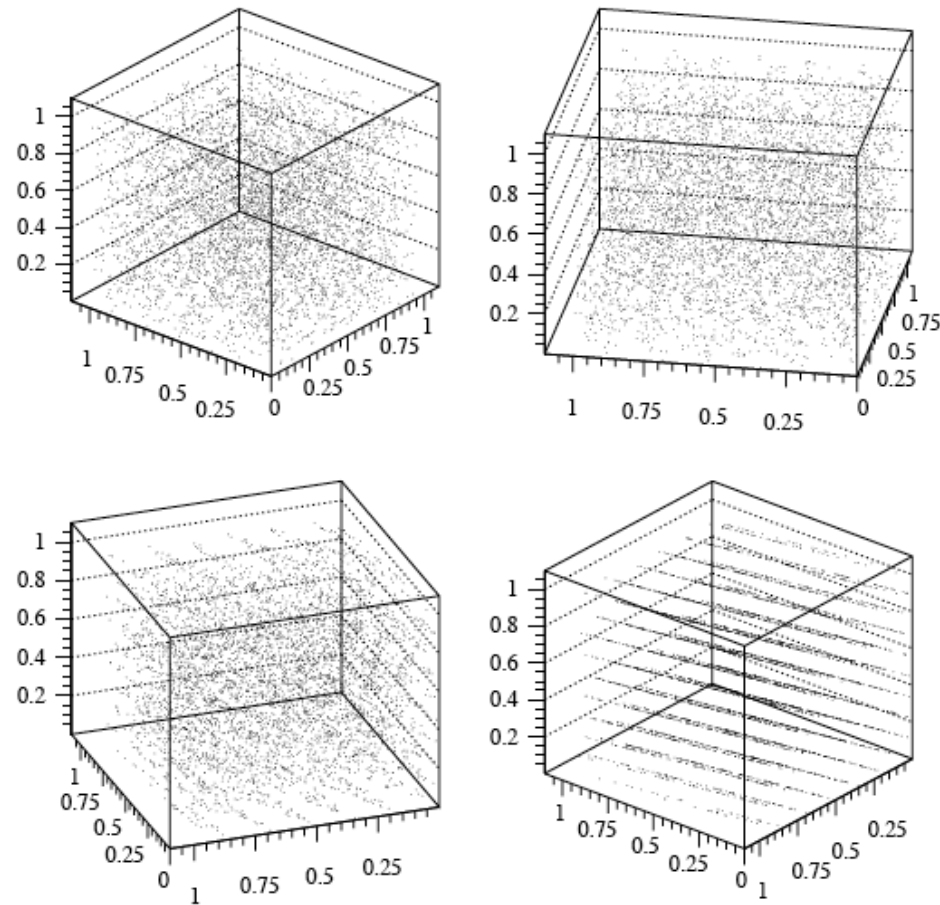
2D distribution Still looks okay

plot pairs: $(\mathbf{x_i}, \mathbf{x_{i+1}})$



plot triplets:

(X_i, X_{i+1}, X_{i+2})



Problem seen when observed at the right angle!

Random numbers fall mainly in the planes

Why? Hint: show that: $x_{k+2} = 6x_{k+1} - 9x_k$

other comments/references on: https://en.wikipedia.org/wiki/Linear_congruential_generator
Also an example of Python code

Problems also with other smart algorithms ...

The authors of *Numerical Recipes* have admitted that the random number generators, RAN1 and RAN2 given in the first edition, are “at best mediocre”.

In their second edition, these are replaced by ran0, ran1, and ran2, which have much better properties.

many editions, see **web site: numerical.recipes;**

free old edition (1996) in fortran:

http://s3.amazonaws.com/nrbook.com/book_F210.html =>

II edition in Fortran90 => B7 Random Numbers p. 1141 or

<http://nrbook.com/a/bookf90pdf.php> => Random number in Ch. 7
(you need the FileOpen plugin for Adobe [Acrobat] Reader®)

Possible improvements

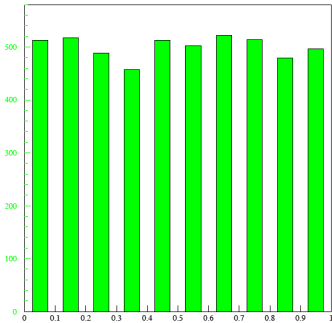
One way to improve the behaviour of random number generators and to increase their period is to modify the algorithm:

$$I_n = (a \times I_{n-1} + b \times I_{n-2}) \bmod m$$

Which in this case has two initial seeds and can have a period greater than m .

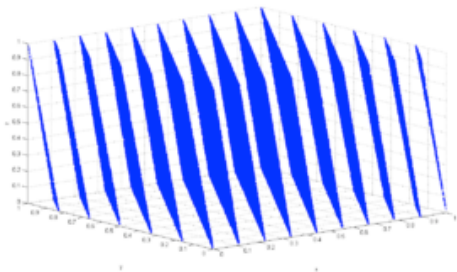
Tests the “quality” of a random sequence

Results from Randu: 1D distribution



- uniformity

(look at the histogram, but also check the moments of the distribution, i.e., $\langle x^k \rangle$, for $k=1, 2, \dots$)



- correlation

- other more sophisticated tests

(in particular for cryptographically secure use!)

Many other (pseudo)random numbers generators

- “Mersenne twister” (Matsumoto and Nishimura , 1997)

The commonly used variant, MT19937, produces a sequence of 32-bit integers with the following desirable properties:

1. It has a very long period of $2^{19937} - 1$ (which is necessary but not sufficient to guarantee of good quality in a random number generator)
2. It passes numerous tests for statistical randomness

- ...

true vs pseudo random number generators

	PSEUDO	TRUE
efficiency	excellent	poor
determinism	deterministic	non deterministic
periodicity	periodic	aperiodic

Technicalities to create our own
(pseudo)random number generator

mod ???

Intrinsic procedures in FORTRAN

(see reference to Chapman book on the moodle page on this Course)

Table B-1: Specific and Generic Names for All Fortran 90/95 Intrinsic Procedures

Generic name, keyword(s), and calling sequence	Specific name	Function type	Section	Notes
ABS(A)	ABS(r) CABS(c) DABS(d) IABS(i)	Argument type Default real Default real Double Prec. Default integer	B.3	2
ACHAR(I)		Character(1)	B.7	
ACOS(X)	ACOS(r) DACOS(d)	Argument type Default Real Double Prec.	B.3	
ADJUSTL(String)		Character	B.7	
ADJUSTR(String)		Character	B.7	
AIMAG(Z)	AIMAG(c)	Real	B.3	
AINT(A, <i>KIND</i>)	AINT(r) DINT(d)	Argument type Default Real Double Prec.	B.3	

...

EXPANDED DESCRIPTION OF FORTRAN 90 / 95 INTRINSIC PROCEDURES

Intrinsic procedures in FORTRAN

(see the page from Fortran90/95 for Scientists and Engineers, by S.J. Chapman)

MOD(A,P)	AMOD(r1,r2) MOD(i,j) DMOD(d1,d2)	Argument type Real Integer Double Prec.	B.3	
MODULO(A,P)		Argument type	B.3	

...

Intrinsic procedures in FORTRAN

MOD(A1,P)

- Elemental function of same kind as its arguments
- Returns the value $\text{MOD}(A,P) = A - P \cdot \text{INT}(A/P)$ if $P \neq 0$. Results are processor dependent if $P = 0$.
- Arguments may be Real or Integer; they must be of the same type
- Examples:

Function	Result
MOD(5,3)	2
MOD(-5,3)	-2
MOD(5,-3)	2
MOD(-5,-3)	-2

MODULO(A1,P)

- Elemental function of same kind as its arguments
- Returns the modulo of A with respect to P if $P \neq 0$. Results are processor dependent if $P = 0$.
- Arguments may be Real or Integer; they must be of the same type
- If $P > 0$, then the function determines the positive difference between A and then next lowest multiple of P. If $P < 0$, then the function determines the negative difference between A and then next highest multiple of P.
- Results agree with the MOD function for two positive or two negative arguments; results disagree for arguments of mixed signs.
- Examples:

Function	Result	Explanation
MODULO(5,3)	2	5 is 2 up from 3
MODULO(-5,3)	1	-5 is 1 up from -6
MODULO(5,-3)	-1	5 is 1 down from 6
MODULO(-5,-3)	-2	-5 is 2 down from -3

mod or modulo
give the same result
if acting on positive
integers

Modulus operator in C++

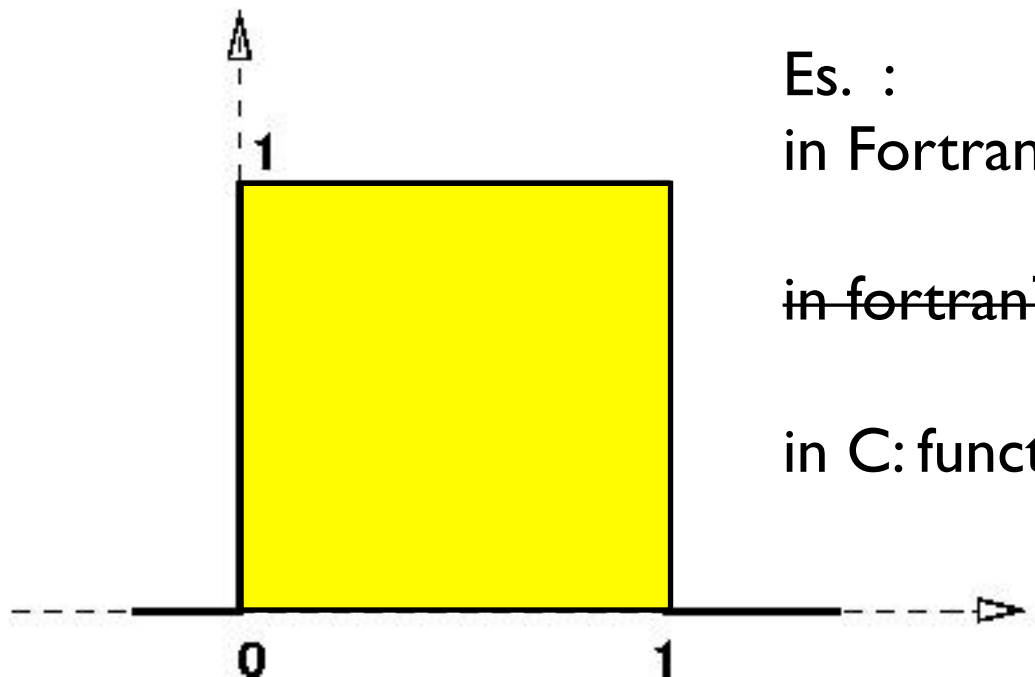
the language provides a built-in mechanism, the **modulus operator** ('%').

Example:

```
01 #include <iostream>
02 using namespace std;
03
04 int main( )
05 {
06     int M = 8;
07     int a = 5;
08     int c = 3;
09     int X = 1;
10     int i;
11     for(i=0; i<8; i++)
12     {
13         X = (a * X + c) % M;
14         cout << X << " ";
15     }
16     return 0;
17 }
```

Intrinsic pseudorandom numbers generators

We could create our own random number generator using “mod” intrinsic function, but it is much better to use directly the (smart) **intrinsic procedures provided by the compilers to generate random numbers,**
in general: real, with uniform distribution in $[0;1[$



Es. :


in Fortran90: subroutine **random_number()**

~~in fortran77: function **drand48()**~~

in C: function **rand** ...

Intrinsic pseudorandom numbers generator in FORTRAN

the name of the produced output has to be specified



RANDOM NUMBER(HARVEST)		Subroutine
RANDOM SEED(<i>SIZE</i> , <i>PUT</i> , <i>GET</i>)		Subroutine

Here (Chapman's book): ARGUMENTS in *Italic* are **optional**
(in other books, optional arguments are in square brackets [])

RANDOM_NUMBER(HARVEST)

- Intrinsic subroutine
- Returns pseudo-random number(s) from a uniform distribution in the range $0 \leq \text{HARVEST} < 1$. HARVEST may be either a scalar or an array. If it is an array, then a separate random number will be returned in each element of the array.
- Arguments:

<u>Keyword</u>	<u>Type</u>	<u>Intent</u>	<u>Description</u>
HARVEST	Real	OUT	Holds random numbers. May be scalar or array.

RANDOM_SEED(SIZE, PUT, GET)

- Intrinsic subroutine
- Performs three functions: (1) restarts the pseudo-random number generator used by subroutine RANDOM_NUMBER, (2) gets information about the generator, and (3) puts a new seed into the generator.
- Arguments:

<u>Keyword</u>	<u>Type</u>	<u>Intent</u>	<u>Description</u>
SIZE	Integer	OUT	Number of integers used to hold the seed (n)
PUT	Integer(m)	IN	Set the seed to the value in PUT. Note that $m \geq n$.
GET	Integer(m)	OUT	Get the current value of the seed. Note that $m \geq n$.

- SIZE is an Integer, and PUT and GET are Integer arrays. All arguments are optional, and at most one can be specified in any given call.

- Functions:

1. If no argument is specified, the call to RANDOM_SEED restarts the pseudo-random number generator.
2. If SIZE is specified, then the subroutine returns the number of integers used by the generator to hold the seed.
3. If GET is specified, then the current random generator seed is returned to the user. The integer array associated with keyword GET must be at least as long as SIZE.
4. If PUT is specified, then the value in the integer array associated with keyword PUT is set into the generator as a new seed. The integer array associated with keyword PUT must be at least as long as SIZE.

warning:
processor-
dependent;
sometimes it
starts always
from
the same
seed !!!

Intrinsic pseudorandom numbers generator in FORTRAN

subroutine **random_number(x)** :

- the argument x can be either a scalar or a N-dimensional array
- the result is one or N *real pseudorandom numbers* uniformly distributed between 0 and 1

subroutine **random_seed([size][put] [get])**

- algorithm is deterministic: the sequence can be controlled by initialization: array of “size” (*) integers (**seed**): different **seeds** -> different sequences

- syntax:

call random_seed(put=seed) to put seed,

call random_seed(get=seed) to get its value

(*): it depends on the compiler (gfortran, g95, ifort, ...) and on the machine architecture

Intrinsic pseudorandom numbers generator in FORTRAN

Further notes:

subroutine **random_number(x)** :

- you can call it directly, without a previous call to random_seed

subroutine **random_seed([size][put][get])**

- all the arguments are optional; i.e., you may also call it as:
call random_seed()

The call without arguments corresponds to different actions, according to the compiler implementation and is processor dependent!!! **check** on your computer!

In some cases it starts always from the same seed, chosen by the computer

Intrinsic pseudorandom numbers generator in C++

real pseudorandom numbers uniformly distributed between 0 and 1:

```
temp = rand();
```

A number between 0 and 50:

```
int rnd = int((double(rand())/RAND_MAX)*50);
```

where RAND_MAX is an implementation defined constant.

Also in c++ the sequence can be controlled by initialization:

```
srand ( time(NULL) );
```


Some programs:

on moodle2.units.it

random_lc.f90

rantest_intrinsic.f90

rantest_intrinsic_with_seed.f90

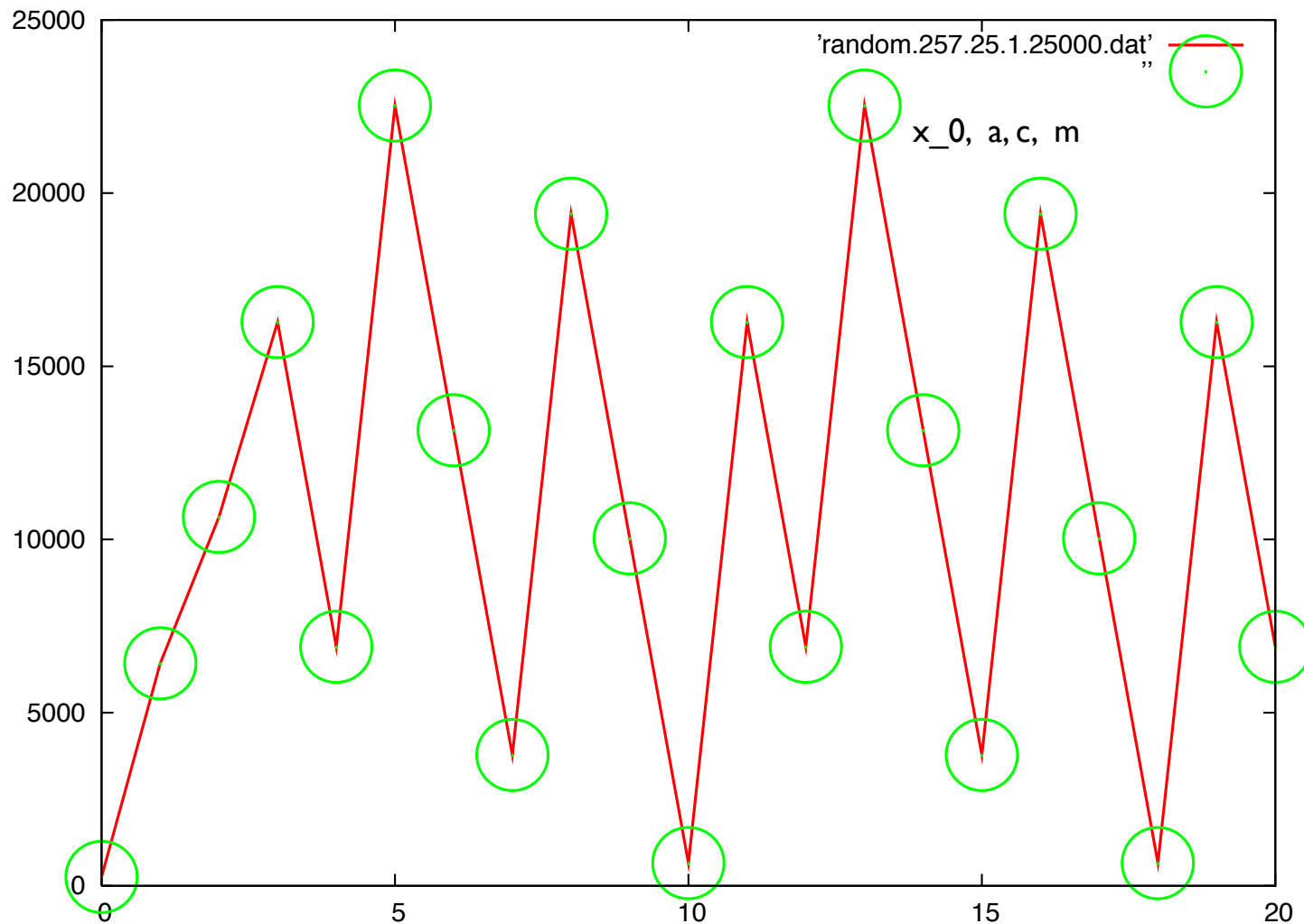
rantestbis_intrinsic.f90

INIT_RANDOM_SEED.f90

nrdemo_ran.f90

Exercise I:

Linear Congruent Method: **periodicity**



How to determine the period “automatically”?

Is it enough to check when a generated number is equal to the initial seed?

NO. In some cases you will NEVER go back to the seed...

A possible algorithm:

- create a sequence of $m+1$ numbers
(you don't need more! why?)
- don't start from the first one, that could be in a transient part of the sequence, but from the last one, which is for sure in the periodic part
- compare all the numbers with the last one, starting from the second to the last and going back by 1 ...
- you get the period!

Exercise 2:

test of **uniformity** of the pseudorandom sequence

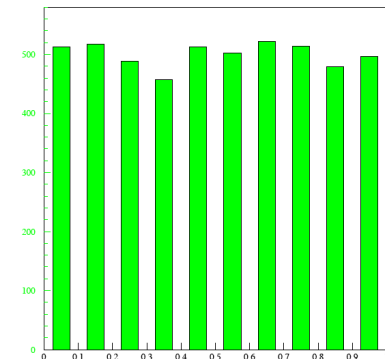
$r(n)$, $n=1, \text{data}$ is our random number sequence between 0 and 1

- (b) Do a histogram with the sequence generated above and plot it using for instance `gnuplot` with the command `w[ith] boxes`. Is the distribution *uniform*?

Hint: to do the histogram, divide the range into a given number of channels of width Δr , then calculate how many points fall in each channel, $r/\Delta r$:

```
integer, dimension(20) :: histog
:
histog = 0
do n = 1, ndata
    i = int(r(n)/delta_r) + 1
    histog(i) = histog(i) + 1
end do
```

Results from Randu: 1D distribution



`<=` counts the number of points falling between $i \cdot \Delta r$ and $(i+1) \cdot \Delta r$ and assign them to the “ $i+1$ ” channel

what is int() ? similar intrinsic functions? how to choose?

AINT(A[,KIND])

- Real elemental function
- Returns A truncated to a whole number. AINT(A) is the largest integer which is smaller than |A|, with the sign of A. For example, AINT(3.7) is 3.0, and AINT(-3.7) is -3.0.
- Argument A is Real; optional argument KIND is Integer

ANINT(A[,KIND])

- Real elemental function
- Returns the nearest whole number to A. For example, ANINT(3.7) is 4.0, and ANINT(-3.7) is -4.0.
- Argument A is Real; optional argument KIND is Integer

FLOOR(A[,KIND])

- Integer elemental function
- Returns the largest integer $\leq A$. For example, FLOOR(3.7) is 3, and FLOOR(-3.7) is -4.
- Argument A is Real of any kind; optional argument KIND is Integer
- Argument KIND is only available in Fortran 95

INT(A[,KIND])

- Integer elemental function
- This function truncates A and converts it into an integer. If A is complex, only the real part is converted. If A is integer, this function changes the kind only.
- A is numeric; optional argument KIND is Integer.

NINT(A[,KIND])

- Integer elemental function
- Returns the nearest integer to the real value A.
- A is Real

what is int() ? similar intrinsic functions? how to choose?

AINT(A[,KIND])

- Real elemental function
- Returns A truncated to a whole number. AINT(A) is the largest integer which is smaller than |A|, with the sign of A. For example, AINT(3.7) is 3.0, and AINT(-3.7) is -3.0.
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NINT(A[,KIND])

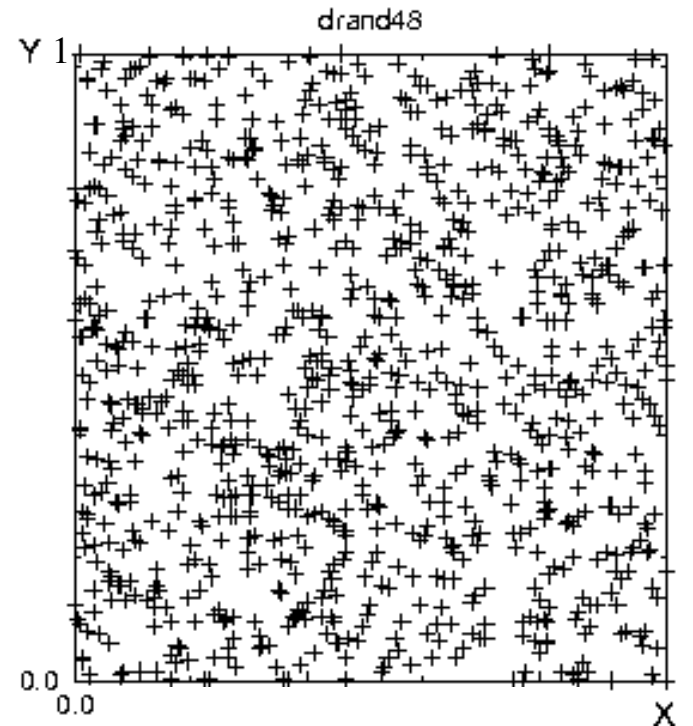
- Integer elemental function
- Returns the nearest integer to the real value A.
- A is Real

Exercise 2:

intrinsic random number generator - test **correlations**

$$(x_i, y_i) = (r_{2i-1}, r_{2i}) \quad i = 1, 2, 3, \dots$$

Testing a Random Number Generator



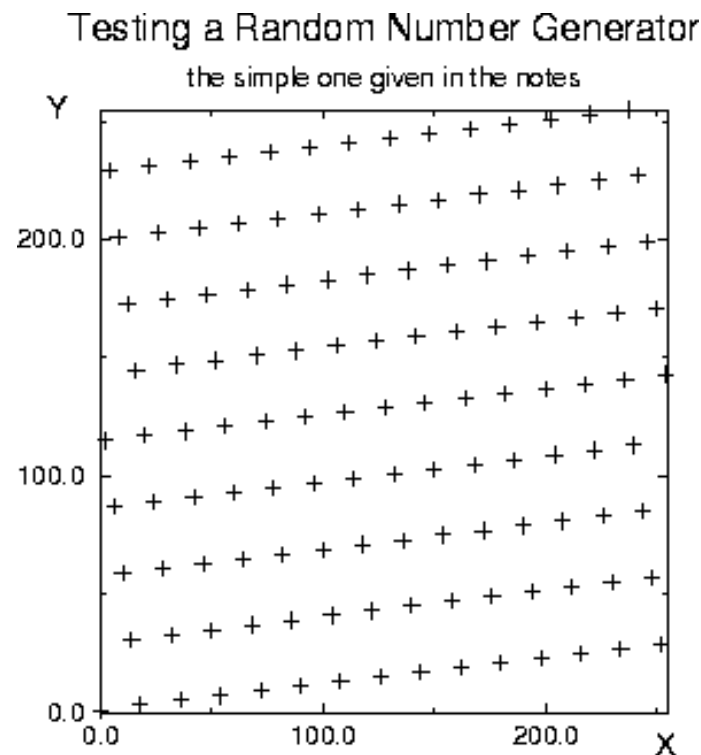
(obsolete: fortran 77)

How many numbers? How many pairs?

but...

correlations with the LCM generator with $M=256$

$$(x_i, y_i) = (r_{2i-1}, r_{2i}) \quad i = 1, 2, 3, \dots$$



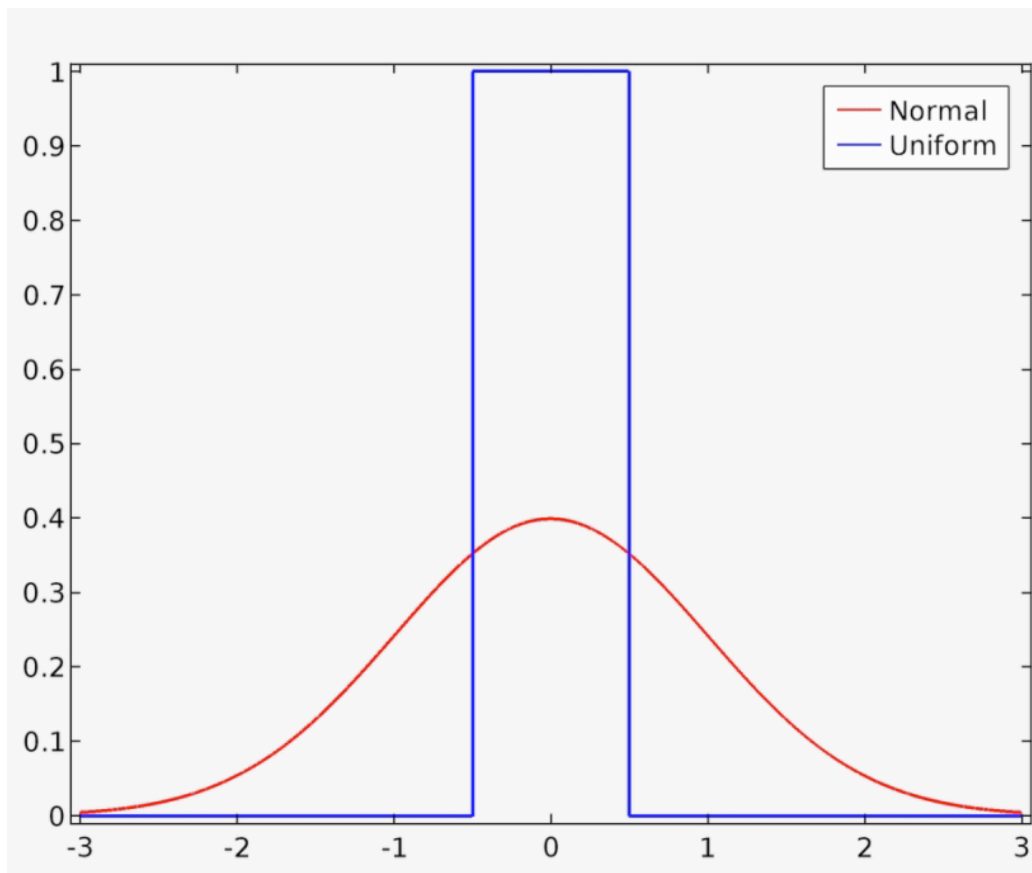
How many numbers? How many pairs?

Exercise 3:

intrinsic random number generator - test **uniformity**

Quantitative tests the “quality”
of a random sequence

two distributions are the same if all the moments $\langle x^k \rangle$ are the same,
and not just the first one $\langle x^1 \rangle$ (average)



e.g.:

uniform and gaussian
distribution centred around
zero have the same average,
but different higher order
momenta

Exercise 3:

intrinsic random number generator - test **uniformity**

(a) For a *uniformity* quantitative test, calculate the moment of order k :

$$\langle x^k \rangle^{calc} = \frac{1}{N} \sum_{i=1}^N x_i^k,$$

that should correspond to

$$\langle x^k \rangle^{th} = \int_0^1 dx \, x^k \, p_u(x) = \frac{1}{k+1}$$

where $p_u(x)$ is the uniform distribution in $[0,1[$. For a given k (fix for instance $k=1, 3, 7$), consider the deviation of the calculated momentum from the expected one: $\Delta_N(k) = |\langle x^k \rangle^{calc} - \langle x^k \rangle^{th}|$, and study its behaviour with N (N up to ~ 100.000). It should be $\sim 1/\sqrt{N}$. (*a log-log plot could be useful*)

$$\text{If } f(x) \sim 1/\sqrt{N} \implies \log(f(x)) \sim -\frac{1}{2} \log(N)$$

A “brute force” test:
Do several
sequences of
different length

```
...
do i=1,N
allocate (rnd(i))
```

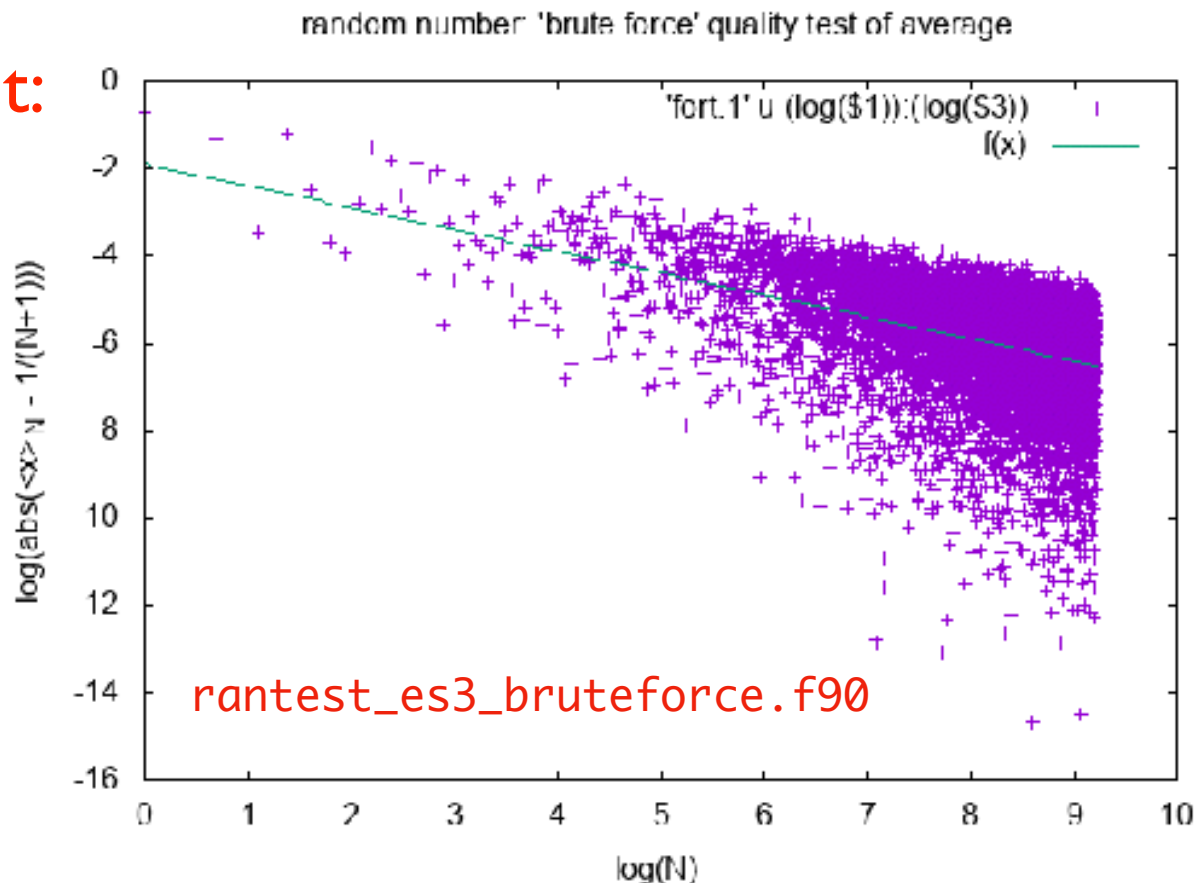
```
call random_number(rnd) ! generate a new sequence of "i" random numbers
                           ! (seed changes automatically)
```

```
somma = sum(rnd**k)  <= this sum() corresponds to an internal loop (nested loops)
```

```
write(1,*)i,somma/i, abs(somma/i - 1./(k+1))
```

```
! somma/i is the PARTIAL sum of the sequence for the momentum k
deallocate(rnd)
```

```
end do
```



ok, but time consuming...

how to calculate the sum of the series for increasing N?

no need of recalculating again the sum from scratch;

print out **partial** sums:

```
implicit none
integer :: N, i, k
real :: sum
real, dimension (:), allocatable :: rnd

print*, ' Insert how many random numbers >'
read(*,*)N
allocate (rnd(N))
call random_number(rnd)

print*, ' Insert the order of momentum >'
read(*,*)k

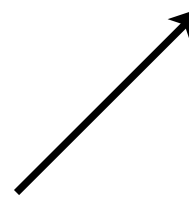
sum = 0.

open (unit=1,file='momentumk.dat')

do i=1,N
sum = sum + rnd(i)**k
write(1,*)i,sum/i, abs(sum/i - 1./(k+1))
! sum/i is the PARTIAL sum of the sequence for the momentum k
end do
```

rantest_es3_simplest.f90

print out the result as a
function of “i”



Test on one sequence, several momenta

rantest_es3_simple.f90

```
...  
allocate (rnd(N))  
call random_number(rnd)  
...  
allocate(sum(kmax))  
..  
sum = 0.
```

```
do k = 1, kmax ! Loop for the different momenta
```


```
do i=1,N  
sum(k) = sum(k) + rnd(i)**k
```

```
write(klabel,*)i, sum(k)/i, abs(sum(k)/i - 1./(k+1))
```

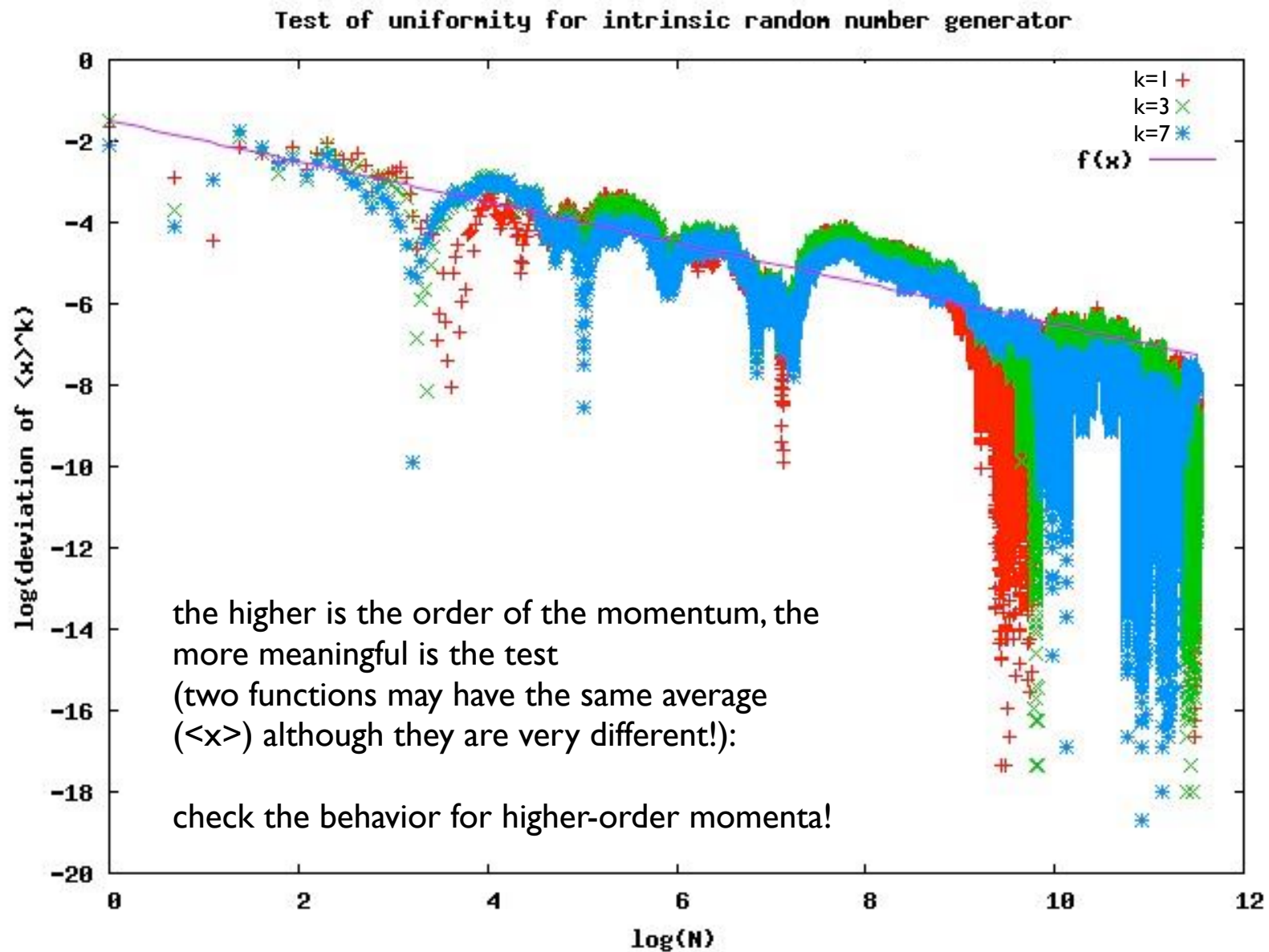
```
! sum(k)/i is the PARTIAL sum of the sequence for the momentum k  
end do ! i
```

```
close(klabel)  
end do ! k
```

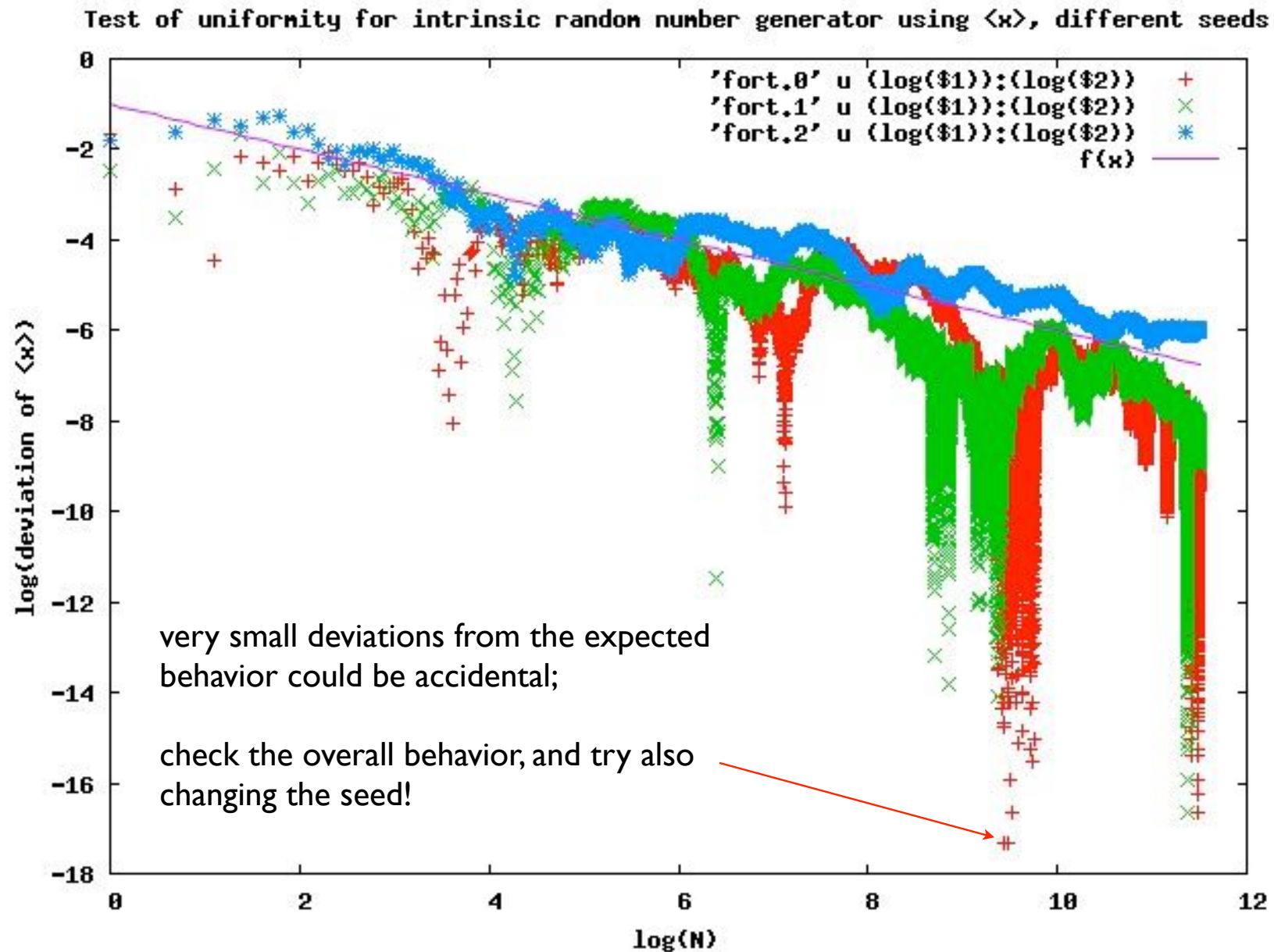
**also here print
the results as a
function of “i”**



Test on one sequence, several momenta



Test on different sequences for a given momentum



A general suggestion:

do you want to check a power law?

$$\text{deviation of } \langle x \rangle^k = \left| \frac{1}{N} \sum_{i=1}^N x_i^k - \frac{1}{k+1} \right| \sim 1/\sqrt{N} + \text{cost.}$$

numerically calculated from the sequence

expected if the sequence was truly uniform

linear regression: much better

$$\log(\text{deviation of } \langle x \rangle^k) \sim -1/2 \log(N) + \text{cost.}'$$

check the slope of the log-log !!!

do you want to fit with gnuplot?

Suppose you have the data in two columns, x and y, and you suspect a power law $y = x^a + \text{const}$

Consider that: $\log(y) = a * \log(x) + b$

```
gnuplot> f(x) = a * x + b
```

```
gnuplot> fit f(x) 'data.dat' u (log($1)):(log($2)) via a,b
```

```
gnuplot> plot f(x), 'data.dat'
```

Exercise 4: use of the seed

integer, dimension(:), allocatable :: seed
integer :: sizer

...

call random_seed(sizer)

! the result depends of the machine architecture!

allocate(seed(sizer))

Check how random_seed() works with **gfortran** or other compilers (**g95**...)
Do you want to force the seed initialization but not “by hands”?

Exercise 5 (optional): how to change the seed using the computer clock

```
SUBROUTINE init_random_seed
  INTEGER :: i, nseed, clock
  INTEGER, DIMENSION(:), ALLOCATABLE :: seed

  CALL RANDOM_SEED(size = nseed)
  ALLOCATE(seed(nseed))
  CALL SYSTEM_CLOCK(clock)

  seed = clock/2 + 37 * (/ (i - 1, i = 1, n) /)
  CALL RANDOM_SEED(PUT = seed)

  DEALLOCATE(seed)
END SUBROUTINE
```

Exercise 6 - optional

nrdemo_ran.f90

```
module ran_module
  implicit none
  public :: ran_func
  contains

  FUNCTION ran_func(idum) result(ran)
    ...
  ...
  END FUNCTION ran_func

end module ran_module
```

```
program demo
  use ran_module
  implicit none
  integer :: i,idum
  real :: x
  print*, "idum (<0) = "
  read*,idum
  x =ran_func(idum)
  ...
end program demo
```

main program & modules

You can:

prepare a module: *modulename.f90*

prepare the main code that uses the module: *mainprogram.f90*

then:

Compile the module with the option -c: this produces .mod and .o (the objects):

```
gfortran -c modulename.f90
```

Compile the main program:

```
gfortran -c mainprogram.f90
```

Finally you link all the files *.o and produce the executable:

```
gfortran -o a.out mainprogram.o modulename.o
```

Data input / output

you can:

prepare an input datafile (say, in.dat)

then:

```
$ ./a.out < in.dat
```

Also the output can be redirected:

```
$ ./a.out > out.dat
```