Numerical Computing - before you start

(General issues, Interpretation of results, potential troubles and traps, etc. ..)

(... strong emphasis on accelerators)

Some (maybe less known) Reading Material

[LL] A.Lichtenberg and M.Lieberman, *Regular and Chaotic Dynamics*, Applied Mathematical Sciences 38, Springer, New York, 1983.

[SC] J.B. Scarborough, *Numerical Mathematical Analysis*, Oxford University Press, Oxford, 1958.

[TF] T. Ferris, *Coming of age in the Milky Way*, HarperCollins, New York, 2003.

[EA] D. Earn et.al. Physica D 56 (1992).

[RN] P. Rannou, Astron. Astrophys. 31, 289.

The purpose of computing for science is insight, not numbers

Dealing with Dynamic Systems it is usually difficult and most likely impossible to find analytical solutions (at least the interestings ones).

The most reliable tools to study Realistic models, e.g. an accelerator, are numerical methods (e.g. amongst others: numerical evaluation of Differential Equations and tracking codes)

- ➡ **Understanding the quality of a numerical method is the key to understand the behaviour of e.g. an accelerators.**
- ➡ **This lecture is not at all meant as an thorough computer science discussion, (i.e. it is liberated from the shackle of a syllabus) rather to cover topics for no more reason that they are interesting and useful**
- ➡ **just writing some code is not enough (by far !)**

Numerical methods have limitations !!

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Numerical methods have limitations !!

Therefore: **"A man's got do know his limitations" (courtesy Dirty Harry)**

If you write complex scientific computer codes and do not take into account the limitations (yours, the computer's and other issues), you will flop !

Therefore: **"A good man always knows his and** his computer's limitations**"**

this we discuss

Discuss and analyse some limitations - Menu

- **Numerical Analysis (can we rely on numbers ?)**
- **Model versus algorithm (do we have a preference ?)**
- **Chaos, (artifical or true ?) and all that ..**
- **Lattice Map (a rescue for some problems ?)**
- **...**

Will touch on a few concepts treated in detail in following lectures, may/should provide some awareness (unlike sometimes said: we shall do more than discussing LINUX versus WINDOWS)

Numerical analysis - (some) typical issues:

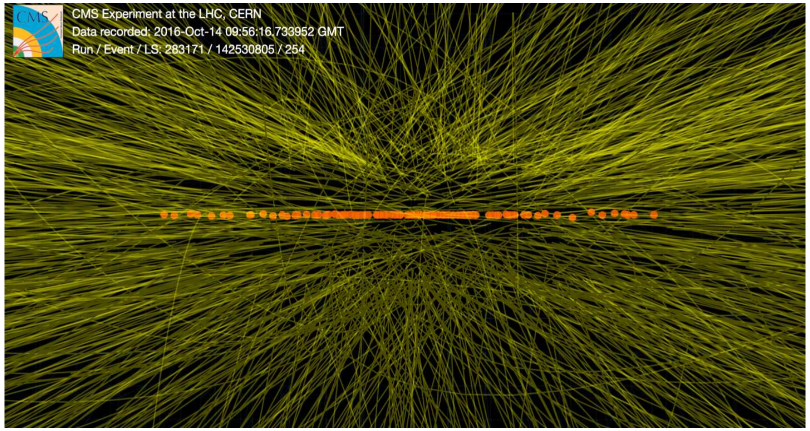
- Intrinsic errors using computers (not programmer's faults)
- Inappropriate algorithms
- Roundoff errors
- Truncation errors
- Conversion errors

Be aware of potential numerical and conceptual difficulties that may exist.

- Numbers are part or the problem, not the answer

Most (if not all) of the following may sound familiar , but the consequences strongly affect the computation and the analysis of the results ! Be prepared and avoid being dogmatic ...

Here is a purpose - challenges for LHC experiments:

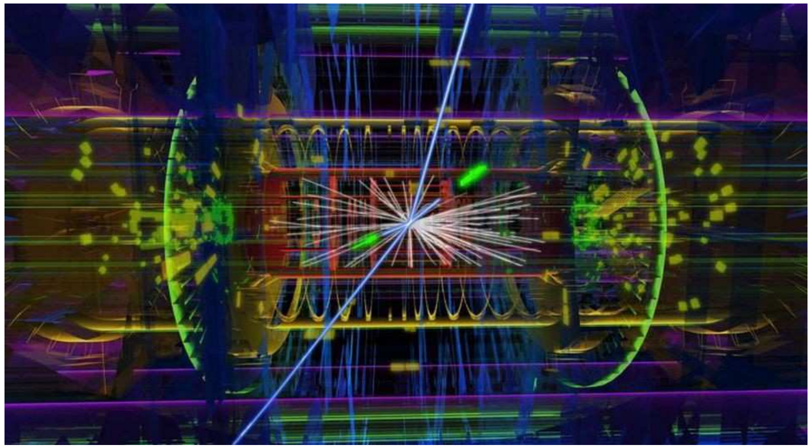


Need to understand what the computer is doing ..

- More than 40 collisions
- Numerically challenging
- Requires careful analysis

Spot the "Higgs"

- Wrong conclusion would be very embarrasing
- Wrong statements are embarrasing



Wrong numbers → wrong conclusions → wrong statements → no price

Numbers (Computers versus mathematicians versus physicists):

Integer, fixed point and floating point (complex ignored for the time being):

- **Integers: usually do not pose any problem:**
  - Unique represention
  - Finite range (due to word length)   Note: starts with 0
- **Fixed point numbers: e.g. 2.71828, 3.14159265*, 299792458.000:**
  - Fixed length (usually linked to word length), machine always keeps the same number of digits, limited range
  - An important use: banking ! (you do not want $16.049999993 \cdot 10^3$ CHF)
  - Fast and easier to implement in hardware (but see later ...)
- **Floating point numbers:**

  Internal representation of floating point numbers use a fixed number of binary digits to represent a decimal number. Some (most) decimal numbers cannot be represented exactly in binary, resulting in problems already for basic operations (addition, subtraction, multiplication, division)

* troubles ahead ..

- **Floating point numbers, some issues:**
  - **So-called scientific notation, e.g. 0.000271828** $\times\ 10^4$**:**
  - **In mathematics, there is a single** 0

    But: $0, \quad -0\,, \quad .000 \times 10^{-9}, \quad .000 \times 10^{+9}$
    are logically the same, but some machines or programming languages make them the same, others do not ! (sometimes for good reasons)
  - **Related:** $1.00 \cdot 10^{-1}$ **and** $0.01 \cdot 10^{1}$ **are stored differently**

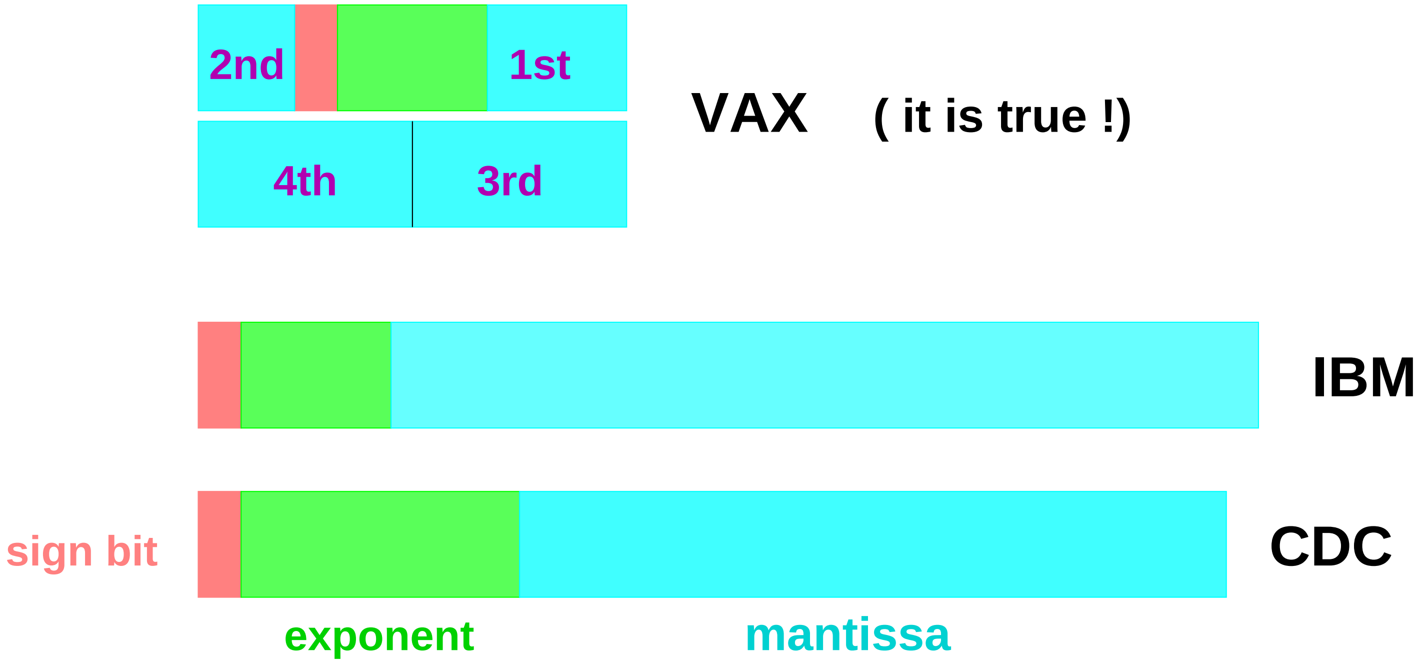
    This has some very unpleasant consequence !
- **<u>Finite arithmetic in mathematics</u> not the same as <u>finite arithmetic of machines</u>**
- **Floating point numbers are a trade-off between range and precision**

  This can/will have strong implications for writing scientific software

First troubles - Floating point Representation on different machines

CERN in the late ’70: mainly 3 types of mainframes; CDC, IBM, VAX

Double precision floating point (64 and 60 bits) representation was:



Exchange of binary floating point numbers somewhat difficult ...

Common standard as defined by IEEE 754 (1985)

Floating point operations can give unexpected results:

0.6/0.2 - 3.0 = -0.44408920985006261617D-15

Equality tests such as (if (x == y) ...) do not work

Another one, we know: $(x+y) \cdot (x-y) = x^2 - y^2$

for x = 0.3 and y = 0.5 we obtain:

$(x+y) \cdot (x-y)$ **= -0.1600000000000000 3109D+00 but**

$(x^2 - y^2)$ **= -0.1600000000000000 0333D+00**

A real good one, try (C or FORTRAN90, float or double, makes no difference):

with: $x = 10^{34}$, $y = -10^{34}$, $z = 1$, $x + (y + z) = ?$ **and** $(x + y) + z = ?$

Try with e.g. C or FORTRAN90 (or any pocket calculator) :

$3.0^{3.0}$ $-3.0^{3.0}$ $3.0^{2.3}$ $-3.0^{2.3}$ $3.0^{-2.3}$ $-3.0^{1.5}$ $-3.0^{0.5}$ $-3.0^{3.1}$

beware of: x^y **!** $\Longrightarrow$ **some are nonsense, some NaN, some are correct ...**

Consider the function:

$$f(x) = \frac{1}{x-1}$$

x	f(x)
1.100000	9.9999976
1.001000	999.9532721
1.000100	9998.3408820
1.000010	99864.380952
1.000001	1048576.000000 I|I
10.100000	0.109890
10.001000	0.111099
10.000100	0.1111098
10.000010	0.1111109
10.000001	0.1111110

well behaved for small changes near $x = 10$

ill-conditioned for small changes near $x = 1$ **(check and avoid)**

Iterative systems - circular accelerators:

The use of computers and numerical methods may require a large number of iterations - typical example simulations for a (circular) machine

- **Iterative systems usually means that results from one stage of the computation are used in subsequent calculations, i.e. a feedback situation**
- **Small errors are propagated and can lead to:**
  - **Loss of precision of the results**
  - **Artifacts leading to wrong conclusions and wrong physics**
- **A powerful tool for (accelerator) simulations but can lead to problems:**

Examples mainly for beam dynamics, but problems can be the same everywhere (some examples later ..)

At every iteration only a fixed number of digits is retained, rounded nearby the representable number. The problems:

- **The "Hamiltonian properties" (see later) are not preserved, can become dissipative hence in the worst case violate Liouville's theorem (see later): worst case scenario ..**
- **For a small number of iterations it is probably not dramatic**
- **The cumulative effect can/will lead to significant changes to the long-term behaviour of e.g. trajectories $\Longrightarrow$ can lead to completely wrong conclusions ..**

The standard argument: use <u>Double Precision</u> and we are save.

Is this always true for practical applications ?

An iterative process IEEE 80 (!) bit precision (both formulae are equivalent):

$$p0 = \frac{1}{\sqrt{3}} \quad \text{and} \quad q0 = \frac{1}{\sqrt{3}} \qquad p_{i+1} = \frac{\sqrt{p_i^2 + 1} - 1}{p_i} \quad \text{and} \quad q_{i+1} = \frac{q_i}{\sqrt{q_i^2 + 1} + 1}$$

with : $6 \cdot 2^i \cdot p^i$	with : $6 \cdot 2^i \cdot q^i$	
0.315965994209750084D+01	**0.315965994209750084D+01**	**Starting point**
0.314271459964536861D+01	**0.314271459964536865D+01**	**Iteration 1**
0.314166274705685013D+01	**0.314166274705684888D+01**	**...**
0.314159703432150639D+01	**0.314159703432152650D+01**	
0.314159292738506092D+01	**0.314159292738509738D+01**	
0.314159267069799892D+01	**0.314159267070199840D+01**	
0.314159265460636674D+01	**0.314159265465930638D+01**	
0.314159265260533476D+01	**0.314159265365663814D+01**	
0.314159264193316416D+01	**0.314159265359005470D+01**	
0.314159264193316416D+01	**0.314159265358979461D+01**	
0.304383829792641763D+01	**0.314159265358979359D+01**	
0.295679307476062510D+01	**0.314159265358979359D+01**	
NaN	**0.314159265358979359D+01**	

Size matters:

Normally 64-bit floating point arithmetic is fully sufficient.

But for numerically sensitive calculations it may be questionable*. May in turn induce other errors: e.g. wrong decision in a conditional branch or real pathological results.

Some examples where higher precision is needed:

- **Supernova simulations (non-local thermodynamic equilibrium)**
- **Climate modelling**
- **Planetary orbit calculation [TF], black hole merger (astrophysicists are smart(er) !)**
- **LHC experiments: Quark, Gluon and Vector Boson scattering. If a phase space point is numerically unstable: recomputed with higher precision**
- **Large matrices (e.g. $n \times n$ with n as large as 10^7) with large condition numbers**

* **most likely insufficient !**

Most programming languages can use arbitrary precision floating point arithmetic using (free) libraries e.g.: popular one for Python is $MPMATH$. Also $ARPREC$ for FORTRAN 90 and C++. UNIX based (also MAC OSX): $MPFUN2015$ for FORTRAN 90 which requires very little changes to existing programs (mainly types).

Some issues:

- **Have to take into account when the code is written: may/does require individual calls to library routines for each arithmetic calculation. Much easier with $MPFUN2015$.**
- **Slow execution time, e.g. rule of thumb compared to 64 bits (17 digits):**
  - **31 digits: $\times$ 5**
  - **62 digits: $\times$ 25**
  - **100 digits: $\times$ 50**
  - **1000 digits: $\times$ 1000**
- **Rather hard to debug**
- **Can cause user fatigue and most scientists give up ... (except maybe a few)**

Better if sufficiently high precision is inbuilt !

Behind your back - Consider the programs:

```c
int main1()
{
double x, y;
x = 4.0/9.0;
y = 8.0/18.0;

if (x == y)
printf("nice");
else
printf("not nice");
}
```

```c
int main2()
{
double x, y;
x = 4.0/9.0;
y = 8.0/18.0;

if (x == 8.0/18.0)
printf("nice");
else
printf("not nice");
}
```

The results ??

Behind your back - Consider the programs:

```
int main1()
{
double x, y;
x = 4.0/9.0;
y = 8.0/18.0;

if (x == y)
printf("nice");
else
printf("not nice");
}
```

```
int main2()
{
double x, y;
x = 4.0/9.0;
y = 8.0/18.0;

if (x == 8.0/18.0)
printf("nice");
else
printf("not nice");
}
```

The results:

- **main1: will always give you nice !**
- **main2: nice or not nice, Hardware and/or Compiler dependent !**

Lesson 1: use a smart compiler with very smart optimizer !
Lesson 2: use it like in main1()

Included datatypes. Furthermore, popular languages, i.e. C++ and FORTRAN 95 and PYTHON allow operator overloading (practical example in the coming few days), this makes it less painful. Examples:

- FORTRAN (95 or higher)
  - Proper Quad Precision (128 bits, up to 62 digits) with e.g.:

    My128 = selected_real_kind(32), My128 is then the TYPE

  - "Quad" Precision (80 bits, up to 62 digits) with e.g.:

    My80 = selected_real_kind(10), My80 is then the TYPE

    For some compilers you can write: REAL*10 and REAL*16 (don't !)
- C/C++
  - VERY compiler and hardware dependent (there is no IEEE standard):

    long double can be anything between 64 and 80 bit precision,
    80 bit is often proper 128 with padding for alignment

    Proper 128 bit with _Quad on Intel compiler
- NO support on Microsoft VC, everything converted to standard double
- Very different for Mathematica, Matlab, etc. ...

Examples, using $1/10$ different languages and types (inbuilt, incomplete):

FORTRAN and C++ single precision:
0.100000001490116120 i.e. 6 - 7 reliable significant digits

FORTRAN and C++ double precision:
0.100000000000000001 i.e. 15 - 16 reliable significant digits

PYTHON double precision (printed using DECIMAL):
0.1000000000000000055511151 i.e. 15 - 16 reliable significant digits

FORTRAN using selected_real_kind(p=18) i.e. 18 significant digits
0.100000000000000000001

Available on some (UNIX !) machines and compilers (e.g. DIGITAL FORTRAN 90)
selected_real_kind(p=33) i.e. 33 significant digits

Mixing different precisions or types: you should know exactly what you are doing !

(e.g. byte streams in communication, TCP)

Use typecasting wherever possible .. (rather good in C++)

Integers have "higher" precision that single floats !!! :

try:

```
#include <stdio.h>
int main(void)
{
   int myint = 16777217;
   float myfloat = 16777216.0;
   printf("my integer  is: %d", myint);
   printf("my float is: %f", myfloat);
   printf("equality ? %d", myfloat == myint);
}
```

Result ?

Integers have "higher" precision that single floats !!! :

try:

```
#include <stdio.h>
int main(void)
{
   int myint = 16777217;
   float myfloat = 16777216.0;
   printf("my integer  is: %d", myint);
   printf("my float is: %f", myfloat);
   printf("equality ? %d", myfloat == myint);
}
```

Result:

my integer is: 16777217
my float is: 16777216.000000
equal ?: 1   (means they are found to be equal)

integer can store 2^{24}**, floating point mantissa is too small (**23**)**

Most problematic: rounding and truncation

Rounding of constants to integers following the IEEE 754 standards:

Mode/Example	5.5	6.5	-5.5	-6.5
to nearest, tied to even	6.0	6.0	-6.0	-6.0
to nearest, tied away from 0	6.0	7.0	-6.0	-7.0
toward 0 (truncation !)	5.0	6.0	-5.0	-6.0
toward $+\infty$ (ceiling)	6.0	7.0	-5.0	-6.0
toward $-\infty$ (floor)	5.0	6.0	-6.0	-7.0

some examples to remember:

1 *float* to *int* causes truncation, i.e., removal of the fractional part.

2 *double* to *float* causes rounding of digit.

3 *long* to *int* causes dropping of excess higher order bits.

After floating point operation:

(63.0/9.) to integer gives: 7
(0.63/0.09) to integer gives: 6

machine dependent !!!

However: Integer to floating point is mostly (!) well behaved

Some computer languages allow to control the truncation/roundoff, e.g. float to integer (C++, FORTRAN 90, Python, ...):

a) Integer part of x (x is truncated)
b) Nearest integer to x (x is rounded)

Some more (no guarantee that it is always true):

Python 3.0 gives: 5/2 = 2.5, 5//2 = 2, 5.0//2 = 2.0

99/3 is float, 99//3 is integer (// means $floor$**)**

FORTRAN 95: 9999999999999999/3 = 3333333333333333
keeps integer (if the result is integer)

Fore some fun: 0.1 is <u>never</u> correctly represented
e.g. with high precision:

0.1 = 0.1000000000000000055511151231257827021181583404541015625
(unlikely to be relevant)

single precision: 0.1 = 0.100000000149011612

Conditional branches make a <u>very</u> big difference whether defined as floating point or fixed point: different use of significant digits !

- **Trouble with small numbers ...**

  subtraction of almost equal numbers may cause extreme loss of accuracy

  → **the most significant digits become 0**

- **Typical example - computing derivatives:**

the derivatives are computed as : $$\frac{f(a+h)-f(a)}{h}$$

For smaller h also $f(a+h)-f(a)$ becomes smaller and makes the least significant digits <u>more</u> important

Side note: programming languages such as C, C++, FORTRAN2003 support infinities - they just follow some rules

a) $+\infty + 5 = +\infty$

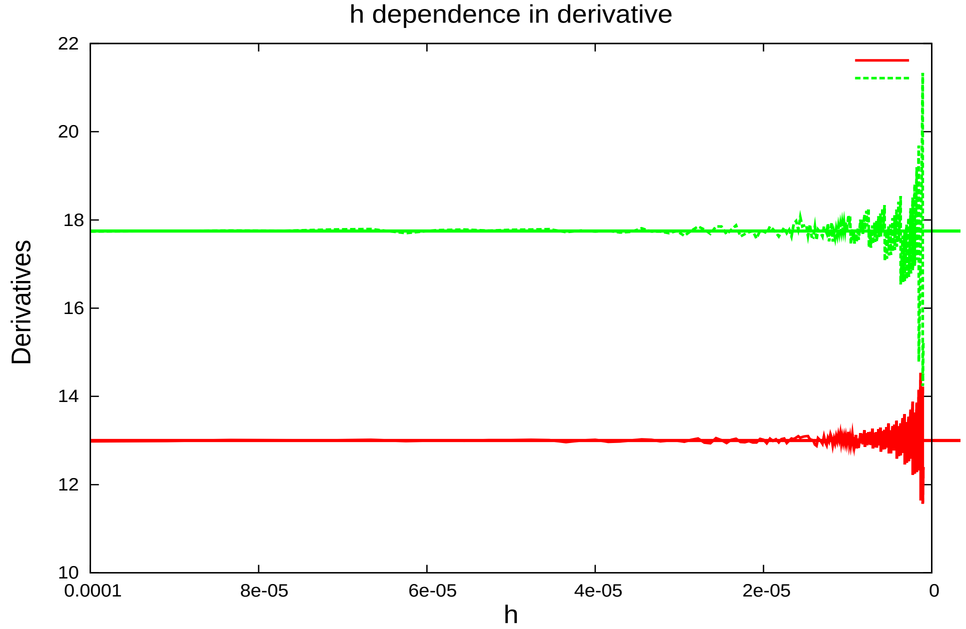
b) $+\infty \times -5 = -\infty$

c) $+\infty \times 0 = NaN$ **(not meaningful)**

Why ? → **they can be used in conditional branches**

$$f(x) = x^2 + \frac{1}{x} + 14x$$

$$f(x) = x^{2.5}$$



the derivatives are computed as : $\dfrac{f(a+h)-f(a)}{h}$

- **For small h the calculation of the derivatives becomes unstable/useless**

  Lesson: avoid subtraction of close numbers !

If you want to do better: wait ..

In this context: A (true !) everyday example - LHC input for a popular optics program:

From database:

```
s.ds.r1.b1:omk,        at= 268.904
mco.8r1.b1:mco,        at= 269.248
mcd.8r1.b1:mcd,        at= 269.2495
mb.a8r1.b1:mb,         at= 276.734
mcs.a8r1.b1:mcs,       at= 284.158
mb.b8r1.b1:mb,         at= 292.394
mcs.b8r1.b1:mcs,       at= 299.818
bpm.8r1.b1:bpm,        at= 300.697
mqml.8r1.b1:mqml,      at= 303.842
mcbcv.8r1.b1:mcbcv,    at= 306.884
mco.9r1.b1:mco,        at= 308.313
mcd.9r1.b1:mcd,        at= 308.3145
mb.a9r1.b1:mb,         at= 315.799
mcs.a9r1.b1:mcs,       at= 323.223
mb.b9r1.b1:mb,         at= 331.459
mcs.b9r1.b1:mcs,       at= 338.883
bpm.9r1.b1:bpm,        at= 339.763
mqmc.9r1.b1:mqmc,      at= 341.739
mqm.9r1.b1:mqm,        at= 345.005
mcbch.9r1.b1:mcbch,    at= 347.346
```

... after "slicing" (sometimes needed, see this afternoon and tomorrow):

s.ds.r1.b1: omk, at = 268.9039999999996
mco.8r1.b1: mco, at = 269.2479999999990
mcd.8r1.b1: mcd, at = 269.249500000000012
mb.a8r1.b1, at = 276.734247349421594
mcs.a8r1.b1, at = 284.158494698843185
mb.b8r1.b1, at = 292.394742048264789
mcs.b8r1.b1, at = 299.818989397686323
bpm.8r1.b1: bpm, at = 300.697989397686342
mqml.8r1.b1..1, at = (303.84298939769) + ((l.mqml) * (0 - 0.333333333333333))
mqml.8r1.b1, at = 303.842989397686324 e.g. its strength: kq8 = -0.00694900907253902
mqml.8r1.b1..2, at = (303.84298939769) + ((l.mqml) * (0.333333333333333))
mcbcv.8r1.b1, at = 306.884989397686354
mco.9r1.b1: mco, at = 308.313989397686328
mcd.9r1.b1: mcd, at = 308.315489397686349
mb.a9r1.b1, at = 315.800236747107931
mcs.a9r1.b1, at = 323.224484096529523
mb.b9r1.b1, at = 331.460731445951126
mcs.b9r1.b1, at = 338.884978795372717
bpm.9r1.b1: bpm, at = 339.764978795372713

comments ??

... after "slicing" (sometimes needed, see this afternoon and tomorrow):

s.ds.r1.b1: omk, at = 268.903999999999996
mco.8r1.b1: mco, at = 269.247999999999990
mcd.8r1.b1: mcd, at = 269.249500000000012
mb.a8r1.b1, at = 276.734247349421594
mcs.a8r1.b1, at = 284.158494698843185
mb.b8r1.b1, at = 292.394742048264789
mcs.b8r1.b1, at = 299.818989397686323
bpm.8r1.b1: bpm, at = 300.697989397686342
mqml.8r1.b1..1, at = (303.84298939769) + ((l.mqml) * (0 - 0.333333333333333))
mqml.8r1.b1, at = 303.842989397686324 e.g. its strength: kq8 = -0.00694900907253902
mqml.8r1.b1..2, at = (303.84298939769) + ((l.mqml) * (0.333333333333333))
mcbcv.8r1.b1, at = 306.884989397686354
mco.9r1.b1: mco, at = 308.313989397686328
mcd.9r1.b1: mcd, at = 308.315489397686349
mb.a9r1.b1, at = 315.800236747107931
mcs.a9r1.b1, at = 323.224484096529523
mb.b9r1.b1, at = 331.460731445951126
mcs.b9r1.b1, at = 338.884978795372717
bpm.9r1.b1: bpm, at = 339.764978795372713

303.842989397686324 is NOT a useful number, in the worst case may lead to problems

It is not just academic (non scientific incidents):

- **1991: Truncation after multiplication of an integer (time) with 0.1 to convert to a floating point number prevented a MIM-Patriot from intercepting a SCUD proposed bug fix: always reboot after 8 hours of operation**

- **1996: ARIANE 5 off trajectory and self-destructed: converted 64 bit float to 16 bit unsigned integer (too large)**

- **1992: Wrong initial report of result from German election (4.97 % rounded to 5.0 %)**

- **1982: Vancouver stock exchange: index from 1000.00 to 520.00 in 2 month (should have been 1100, after each transaction the value was not rounded but truncated)**

- **2025:**

Discussion 1:

- **Be aware of (unavoidable) numerical problems**
- **Avoid being dogmatic: problems are intrinsic, the choice of your favorite operating system or programming language does not help at all (the issues may even be different and re-writing can become tricky) : it is not the ink that makes the splotches**

This means that programmers need to implement their own method of detecting when they are approaching an inaccuracy threshold, must guard against it at all times !
Or else give in the quest for a robust, stable implementation of an algorithms.

Some algorithms can be scaled so that computations don't take place in the constricted area near problems. However, scaling the algorithm and detecting the inaccuracy threshold can be difficult and time-consuming for each numerical problem.

Next: implications for interpretation of beam dynamics calculations →

Terms important for dynamics (stability) of particles - stochastic versus chaotic behaviour

Confusion alert → they may appear equivalent from the point of view of an observer, but are totally different phenomena:

- **Stochastic motion is random at all times and all amplitudes**
- **Chaotic motion is predictable in the short term, but can appear random at longer time and periods of an iterative system. At long term because it is very sensitive to initial conditions and intrinsic to the dynamics, usually depends on particle amplitudes (dynamic aperture)**

To determine a "dynamic aperture" (see other lectures) stochastic contributions should be avoided and are often due to one of these problems:

- **Random by construction (e.g. "Monte Carlo" simulations)**
- **Random due to external noise (e.g. power converters, vibrations, ...)**
- **Numerical noise, in particular truncation or rounding**

"Chaotic behaviour" is what we may want to study/observe

Some of our main interests:

- Is the machine stable ?
- Do we observe chaos (of the motion) ?

If we do "observe" chaotic motion:

- Chaotic motion should be intrinsic to the dynamics and not the result of numerical artifacts associated with finite precision arithmetic
- Can easily be due to a not absolutely exact method of integration

Key: need an unambiguous understanding of a physical mechanism and whether this mechanism really accounts for the observed chaos

The underlying model (e.g. the description of the machine, no need for attometer precision) can be an approximation (which is always the case !), the algorithm must be exact (within the limitations of the computer itself, i.e. truncation errors etc.).

Some keywords here, the gory details in other lectures: Hamiltonians, symplecticity, Lie integrators, lattice maps, ...

Anticipating a following lecture, a key issue for the stability of a simulation (in particular iterations) is the concept of symplecticity (will come many times).

Symplecticity in a nutshell (consider a pendulum):

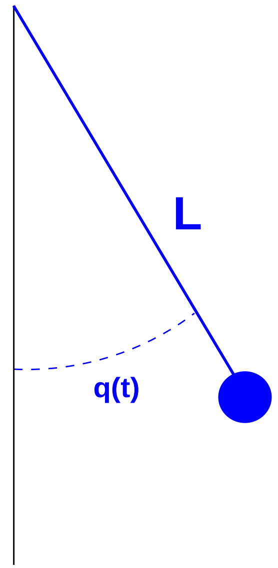
Equation of motion (2D):

$$\ddot{q}(t) = -\frac{g}{L} \cdot \sin(q(t))$$

Reduce to 2 equations 1D:

$$\dot{q}(t) = v(t)$$

$$\dot{v}(t) = -\frac{g}{L} \cdot \sin(q(t))$$



1. Break time t into steps Δt: $\rightarrow \quad t_k = k \cdot \Delta t$ "time" is now a discrete variable t_k
2. $q(t) \rightarrow q_k$ and $v(t) \rightarrow v_k$
3. Solve for q_{k+1} and v_{k+1} (various methods)

Method 1 (fast, unstable, bad accuracy, energy blows up):

$$
\begin{aligned}
q_{k+1} &= q_k + \Delta t \cdot v_k \\
v_{k+1} &= v_k - \Delta t \cdot \frac{g}{L} \cdot \sin(q_k)
\end{aligned}
$$

Method 2 (stable, slow, bad accuracy, energy dissipative):

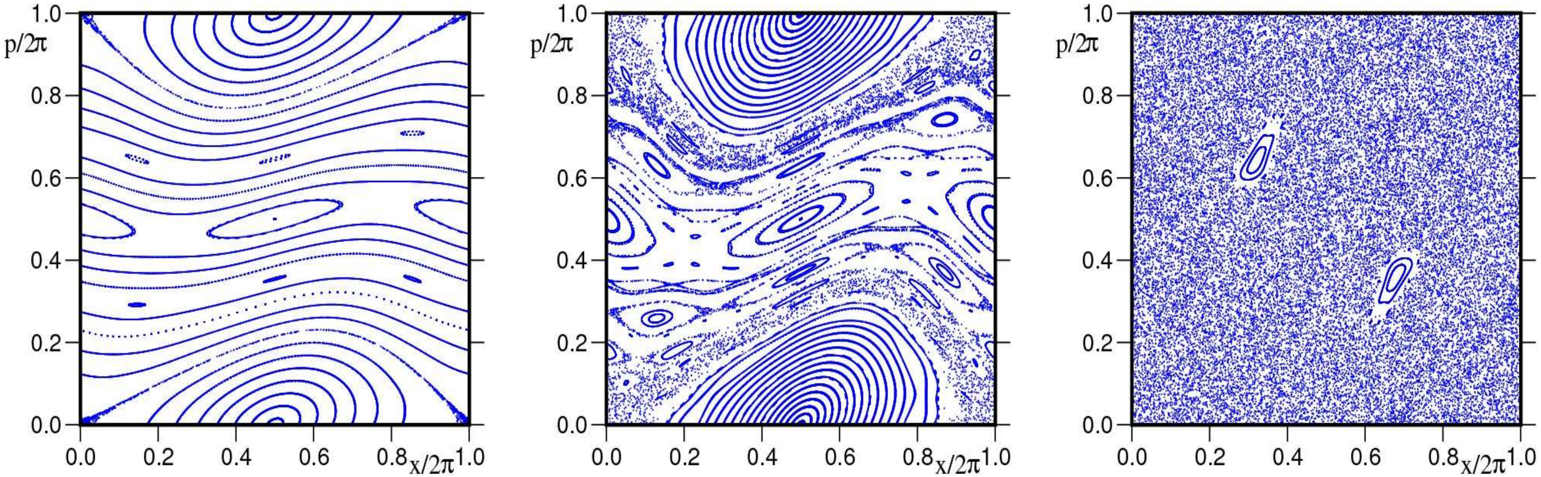
$$
\begin{aligned}
q_{k+1} &= q_k + \Delta t \cdot v_{k+1} \\
v_{k+1} &= v_k - \Delta t \cdot \frac{g}{L} \cdot \sin(q_{k+1})
\end{aligned}
$$

Method 3 (stable, good accuracy, energy conserved, symplectic):

$$
\begin{aligned}
q_{k+1} &= q_k + \Delta t \cdot v_{k+1} \\
v_{k+1} &= v_k - \Delta t \cdot \frac{g}{L} \cdot \sin(q_k)
\end{aligned}
$$

The third is the best known (Hamiltonian) map and is called the "standard map"

Dealing with the standard map (plotted in Phase Space - x versus p_x:



K = 0.50 K = 0.97 K = 2.00

The behaviour, e.g. regular or chaotic motion depends on the parameter $K = \frac{g}{L}$

Transition to chaotic/stochastic layers appear for K = 0.97

However, for studying very long term behaviour: due to roundoff or truncation errors, the standard map will <u>always</u> produce some chaos.

How to detect chaotic behaviour ?

A standard procedure: evaluate Lyapunov exponent, e.g. [LL]

"It characterizes the rate of separation of initially infinitesimally close (!) trajectories"

→ a measure for the stability of a dynamic system, therefore a critical parameter to be evaluated

It cannot be computed analytically, hence must rely on numerical techniques.

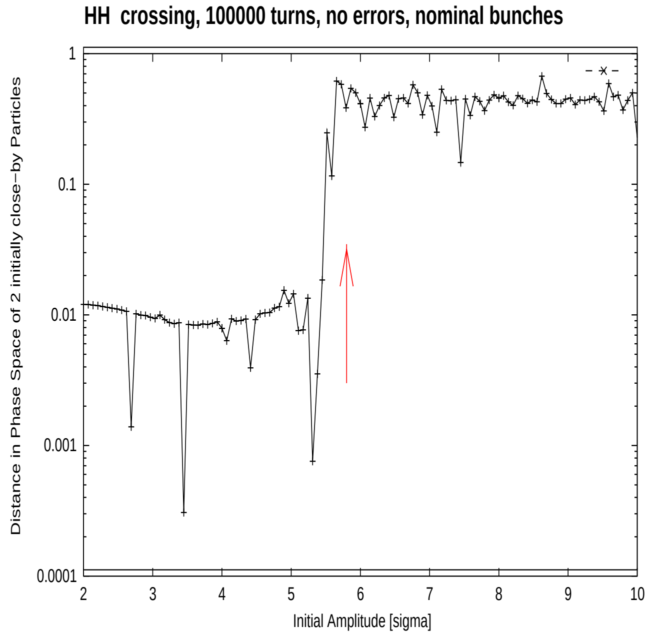
Typical use in accelerator design: single particle tracking to estimate region of stability of trajectories (dynamic aperture). In the long term particles can "slip" into chaotic region.

→ Track two particles initially very close in Phase Space and see what happens ...

LHC with two beam-beam interactions

Two particles started very close in Phase Space

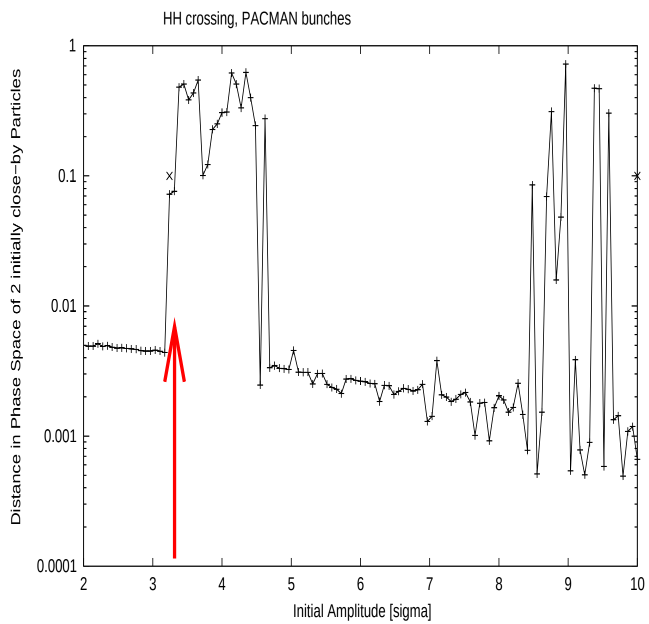
Plotted:
Phase Space distance after tracking 10^5 iterations (turns, corresponds to $\approx 10^9$ machine elements in this case)



Phase Space distance between the particles "jumps" by 2 orders of magnitude (and stays up)
Depends only on particle amplitudes (in this example $\approx$ 6 σ) ➡ clear evidence for onset of chaotic behaviour - in this case cross-checked with another parameter

The physics:
nonlinear beam-beam interactions make particles unstable at large amplitudes

Another example:



Again: LHC with two **beam-beam** **interactions (but different parameters)**

An unstable "band" followed by a "stable region"

The corresponding Phase Space structures can be reproduced (maybe in another lecture)
Depends only on particle amplitudes (in this example $\approx 6\ \sigma$) ➡ clear evidence for onset of chaotic behaviour - in this case cross-checked with another parameter

The physics:
nonlinear beam-beam interactions make particles unstable at large amplitudes, but hit a resonance at smaller amplitudes, then stable again

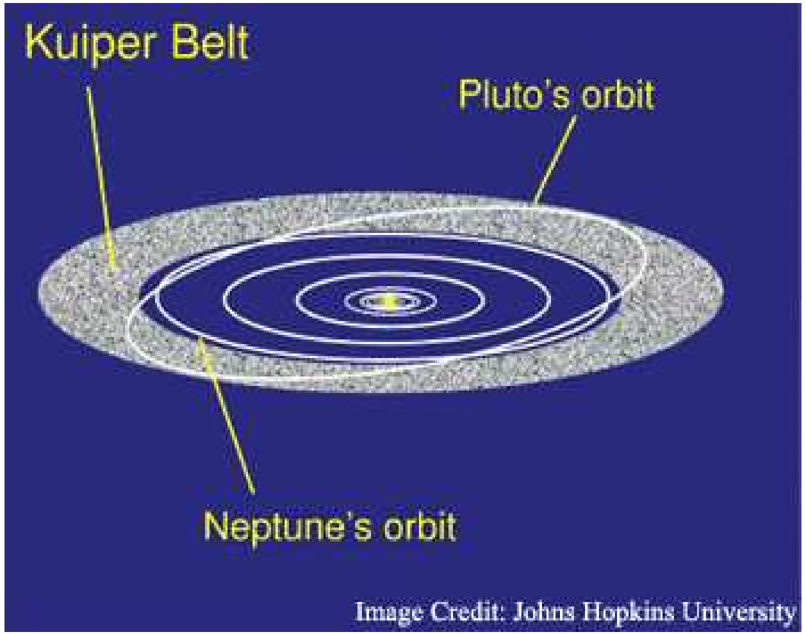
Not just accelerators - largest chaotic system: Solar System

Pluto: orbit highly inclined and eccentric (crosses the Neptune orbit !)

Motion chaotic (but not unstable) due to resonance with Neptune

Maybe also exhibit "stable bands" ! (beyond Saturne)

Requires N-body simulation (long term, over Myrs or Gyrs)



Problems very similar to beam stability: chaos, roundoff, symplecticity, etc. Can we profit from those studies ?

"Exact Numerical Studies of Hamiltonian Maps, Iterating without roundoff Errors", D. Earn et.al. Physica D 56 (1992)

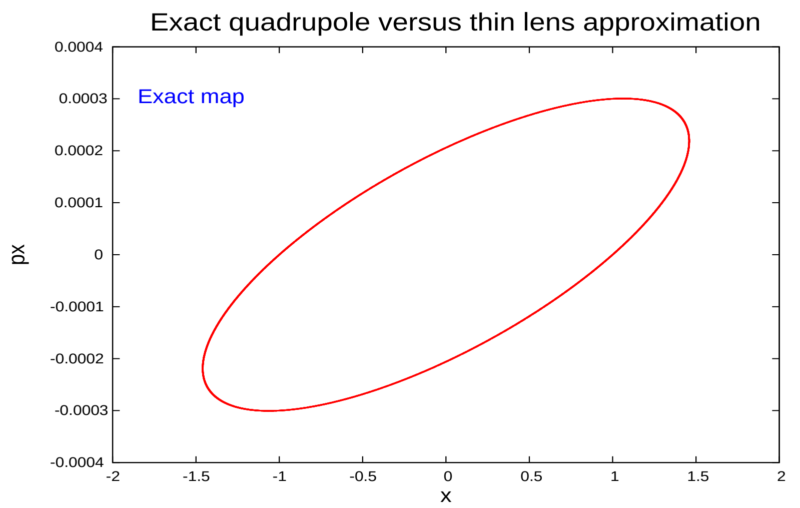
→ last part of this lecture ...

How does this relate to a (circular) accelerator ?

Take the most trivial example: Linear Motion in 1D (remember High School)

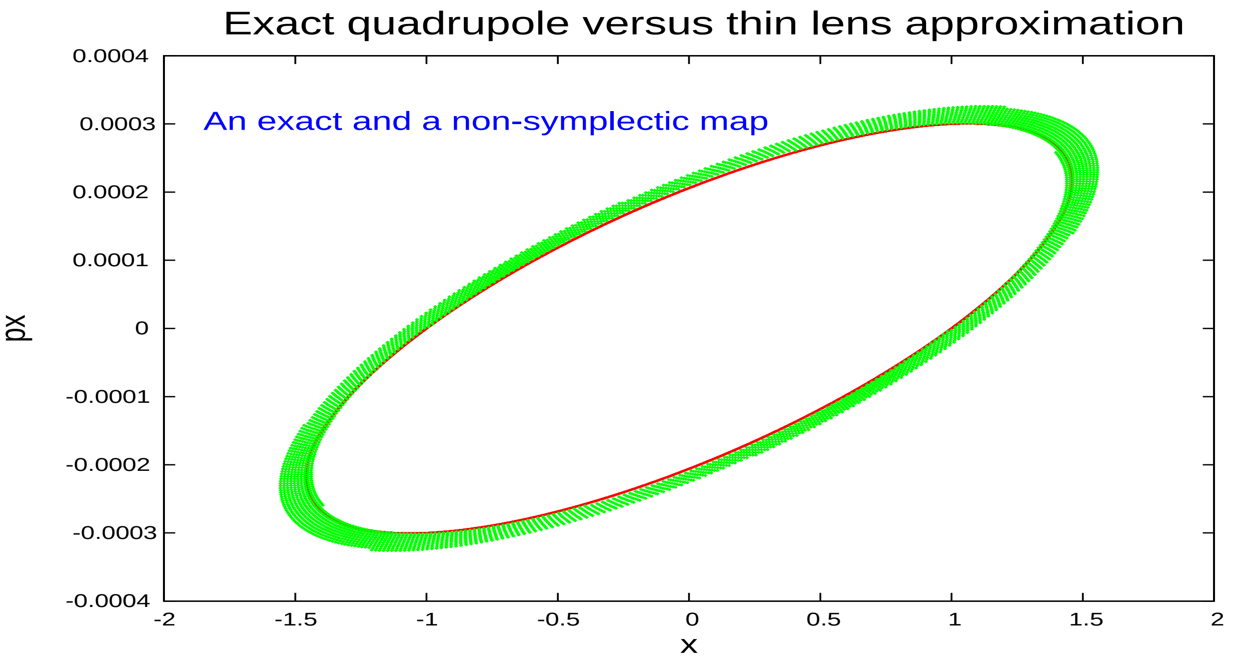
➡ **Consider one turn as a time step for this exercise (in reality the machine is split into many time steps around the whole machine, but the arguments don't change)**

Plotting the variables (now x and p_x) once per turn (again see later lecture) one gets an ellipse in phase space:



The <u>exact model</u> of the machine and <u>exact algorithm</u> are used

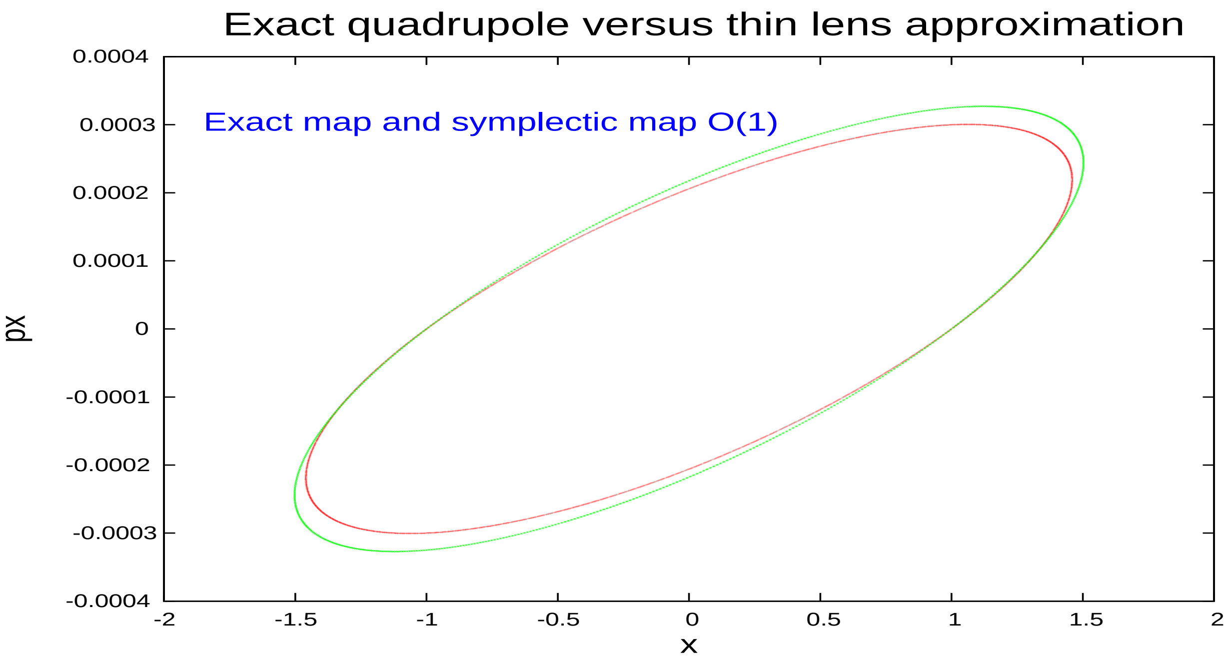
A non-symplectic solution



Non-symplecticity: particles spiral towards outside (could also go to the inside), artifact of the algorithm

- **<u>exact model</u>, but <u>approximated algorithm</u>**
- **drawing conclusions from that is totally careless (but frequently happens)**
- **the lesson: make sure the physical mechanism can be explained**

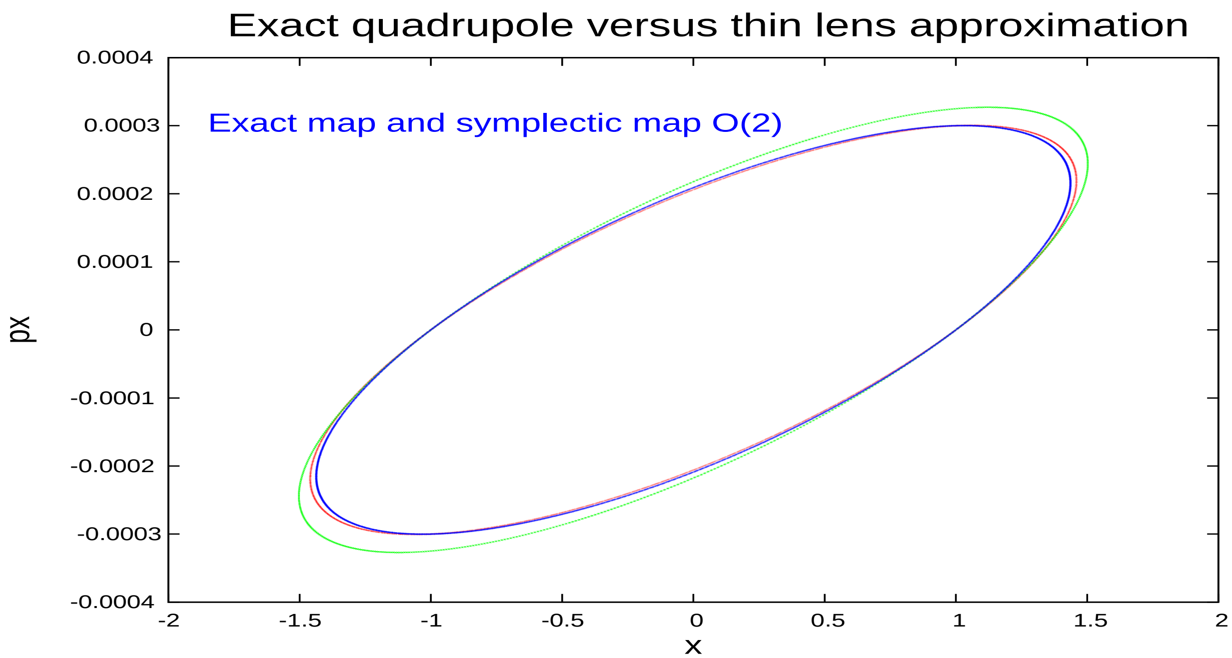
Symplectic solution, model is $\mathcal{O}(L^1)$



symplectic, i.e. exact integrator, visible inaccuracy but the physics is right

→ **model slightly approximated $\mathcal{O}(L^1)$, algorithm exact**

Symplectic solution, improved model ($\mathcal{O}(L^2)$)



symplectic (in theory), solution with model order $\mathcal{O}(L^2)$, but already good accuracy

Lesson from that → different cases:

- **Model approximate and algorithm approximate**
- **Model exact and algorithm approximate**
- **Model approximate and algorithm exact**
- **Model and algorithm exact**

Only the two latter are acceptable, otherwise the physics stinks

There is no general remedy to improve approximate models but errors due to approximate algorithms should be made as small as possible.

Back to the standard map:

Is it possible to avoid truncation and roundoff errors ?

For very long term tracking (e.g. Gyrs) eventually one is beaten by truncation and roundoff errors - all machines are finite ..

Are there any numbers not (or less) troubled by these (unavoidable) errors?

- **For Fixed Point numbers bits are eliminated, but some rounding is done <u>before</u> the elimination. Better than just truncation.**
- **All integer numbers: They are limited by the number of bits, but no truncation or roundoff. No chaos or stochastic behaviour can come from numerical artifacts.**

But can Integer Numbers be used for anything useful ?

Prerequisites: integration technique, method 3

It is usually used to integrate trajectories for a Hamiltonian like: $H = \frac{1}{2}v^2 + U(x,t)$

$$x(t+\Delta t) = x(t) + \Delta t \cdot x'(t+\Delta t)$$

$$x'(t+\Delta t) = x'(t) + A \cdot \Delta t \cdot x(t)$$

A **is the force derived from the potential:** $A = -\nabla U(x,t)$

To "cure" the truncation errors: multiply the potential by a (periodic) time dependent factor with average zero:

$$\tilde{H} = \frac{1}{2}v^2 + U(x,t) \cdot \sum_n \delta(t - n \cdot \Delta t)$$

First → introducing Lattice Maps:

Usually one uses floating point maps:

$$
\begin{aligned}
x_{n+1} &= x_n + something \\
y_{n+1} &= y_n + something
\end{aligned}
$$

The time dependence of x and y is continuous.

Lattice maps:

- Each element is set on a lattice with given dimension
- Map: time is discrete
- Lattice: space is discrete

Solving Differential equations often using this procedure

Replace time step by finite, discrete steps

$$x_{n+1} = x_n + \underbrace{\Delta t \cdot x'_{n+1}}_{drift}$$

$$x'_{n+1} = x'_n + \underbrace{A \cdot \Delta t \cdot x_n}_{kick}$$

It can be considered as a sort of "kick" and a "drift" and A is the force derived from the potential: $A = -\nabla U(x,t)$

Now going for the roundoff error ➡ Integer Lattice maps [EA, RN]

After change of scale, lattice points have integer coordinates, iterations are done without error

The scheme is now: the function Ψ itself is <u>discretized</u> onto a lattice with:
Integer Grid Points (m, n) → lattice points have Integer Coordinates !.

Integer coordinates do the iterations on the nodes without rounding errors.

The nodes are separated by Δx and $\Delta x'$. Each node has a value $\Psi(m, n)$ of the distribution function.

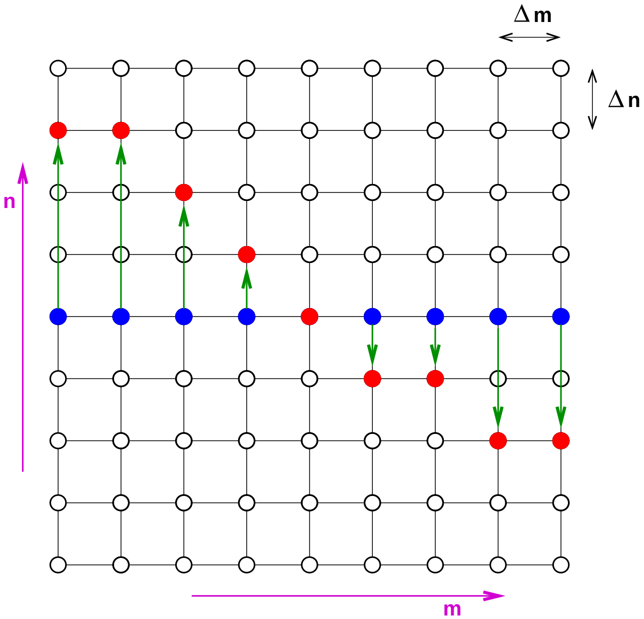
Important: for a lattice with m points per unit, the time step Δt must be choosen so that $m \cdot \Delta t$ becomes an integer.

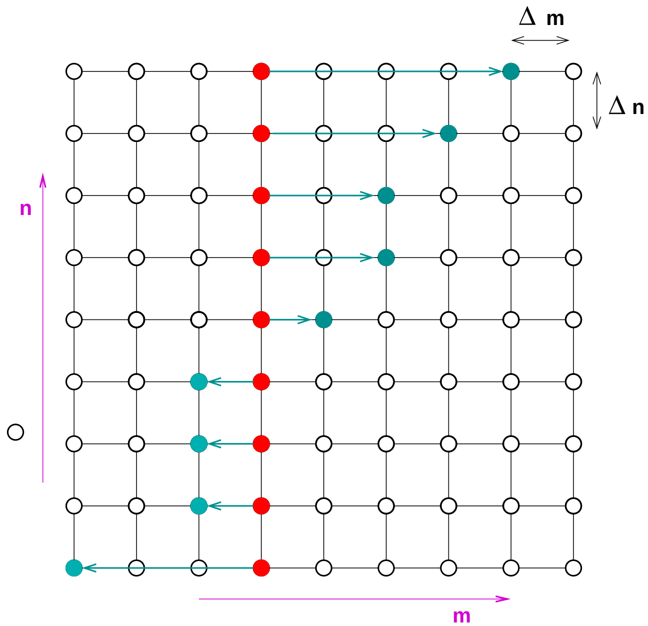
The procedure "shifts" particles on the lattice (from one lattice point to another).

With each time step Δt the value $\Psi(m, n)$ is updated to a new lattice node using a "kick" and "drift" step, i.e.

$n + [\Delta t \cdot A] \rightarrow n$ followed by $m + [\Delta t \cdot n] \rightarrow m$

Each node represents a point in Phase Space (not necessarily a single particle)





With each time step Δt the value $\Psi(m,n)$ is updated to a new lattice node using a "drift" and "kick" step, i.e.

$n \; + \; \lfloor \Delta t \cdot A \rceil \quad \rightarrow \quad n$ ”kick”, left picture

$m \; + \; \lfloor \Delta t \cdot n \rceil \quad \rightarrow \quad m$ ”drift”, right picture

$X_n, \; Y_n$ **are integers.** **Note: $\lfloor ... \rceil$ is the operator: "rounding to nearest integer"**

Discussion 2:

- **The update steps are first order, prior to rounding**
- **The method has no rounding errors**
- **The limit of a continuous floating point map is approached for increasing resolution, i.e. large n and m**
- **Uneffected by round off: The integration scheme is fully reversible.**

➤ **This "tracking" is not fully exact (for finite n and m), but <u>DOES NOT</u> produce numerical artifacts such as (wrongly interpreted) chaotic behaviour**

➤ **Their use has practical value when systems are studied over long time scales**

➤ **It is <u>exactly</u> Hamiltonian, i.e. for example: phase space trajectories cannot intersect.**

As practical example: using the "standard map"

Written in a general form (method 3):

$$x_{n+1} = x_n + y_{n+1}$$

$$y_{n+1} = y_n + \frac{K}{2\pi} \sin(2\pi x_n)$$

Step 1: Replacing the variables x **and** y **and the standard map becomes:**

$$x \Longrightarrow X = m \cdot x$$

$$y \Longrightarrow Y = m \cdot y$$

it can be written as

$$X_{n+1} = X_n + Y_{n+1}$$

$$Y_{n+1} = Y_n + \frac{m \cdot K}{2\pi} \sin(\frac{2\pi}{m} X_n)$$

Step 2: Replace $\frac{m \cdot K}{2\pi} \sin(\frac{2\pi}{m} X_n)$ **by a function** $S_m(X)$ **to take integer values on the lattice points:**

$$S_m(X) = \left\lfloor \frac{m}{2\pi} K \sin\left(\frac{2\pi}{m} X\right) \right\rceil \quad \text{where X is an integer}$$

with that, the new mapping becomes:

$$\begin{pmatrix} X_{n+1} \\ Y_{n+1} \end{pmatrix} = I_m \begin{pmatrix} X_n \\ Y_n \end{pmatrix} = \begin{pmatrix} X_n + Y_n + S_m(X_n) \\ Y_n + S_m(X_n) \end{pmatrix}$$

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But there is one obvious question/problem !

Step 2: Replace $\frac{m \cdot K}{2\pi} \sin(\frac{2\pi}{m} X_n)$ **by a function** $S_m(X)$ **to take integer values on the lattice points:**

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It is a coarse-grained model and assuming $m = n$ **there is only a <u>finite number</u> of system states:** m^2 **!**

➡ **after** $\leq m^2$ **iterations the system must returned to a state already visited before, therefore all trajectories are periodic.**

Seems we have avoided rundoff and truncation errors, but cannot distinguish between chaotic and regular motion !!! Looks like a real flop ...

Any hope ?

Without proof (For examples and details see [LL], [RN]):

One can assume for a given map that we have regular (e.g. showing up as ellipses) and non-regular behaviour (see standard map for K around 0.97)

One can "compare" with a "normal" tracking with the following findings:

The (suspected) system states (X, Y) have extremely long periods filling more evenly the space around "stable ellipses". It is legitimate to assume that they characterize chaotic motion.

Prove for yourself: there are $M!$ ($M = m^2$) possible one-to-one mappings of the $n \times n$ grid onto themselves.

Attribute the same probability $\frac{1}{M!}$ for each of the $M!$

It can be shown [RN] that (here basics only):

1. **Probability for a <u>cycle</u> of "length" n iterations from some point (X, Y) is $\frac{1}{M}$ and does not depend on n**
2. **Average length <n> is about $\frac{1}{2}(M + 1)$**

This is strongly supported by numerical experiments

- **One can avoid roundoff and truncation errors using Integer maps**
- **Criteria for random or chaotic behaviour are defined and are at least as good as standard procedures, without the danger of rounding or truncation errors**

SUMMARY

- Before some calculations: anticipate possible sources of problems, good algorithm design and the implementation of these algorithms must be the main issues right at the beginning. It is a mistake to believe these issues can be solved at the end of the software development cycle.
- Reading the code may not be sufficient to predict the outcome and no guarantee that the same procedures (or algorithms) give the same results every time and on every platform
- Choice of operating system and/or programming language is much less important. All platforms and languages have sweet spots and weaknesses. Largely depends on purpose and required performance:
  → A program with 400 000 lines of code has different needs than a web interface, a device driver or the need for a rapid application development. Some languages emphasize the role of the computer, others the role of the programmer
- Look around what people in other fields are doing and always use computer number 1

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Thanks for attention and have fun at the school ...

- BACKUP SLIDES -

Floating point operations can give unexpected results:

0.6/0.2 - 3.0 = -0.44408920985006261617D-15

Equality tests such as (if (x == y) ...) do not work

Another one, we know: $(x+y)\cdot(x-y) = x^2 - y^2$

for x = 0.3 and y = 0.5 we obtain:

$(x+y)\cdot(x-y)$ = **-0.1600000000000000 3109D+00** **but**

(x^2-y^2) = **-0.1600000000000000 0333D+00**

A real good one, try (C or FORTRAN90, float or double, makes now difference):

with: x = 10^{34}, y = -10^{34}, z = 1, x + (y + z) = 0 **and** (x + y) + z = 1

Try (with C or FORTRAN90):

$3.0^{3.0}$ $-3.0^{3.0}$ $3.0^{2.3}$ $-3.0^{2.3}$ $3.0^{-2.3}$ $-3.0^{1.5}$ $-3.0^{0.5}$ $-3.0^{3.1}$

beware of: x^y **!** $\Longrightarrow$ **some are nonsense, some NaN, some are correct ...**