

How Computers Handle Numbers

A.k.a. Computer Arithmetic Uncovered

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Stratospheric Overview

Integers (\mathbb{Z}), reals (\mathbb{R}) and complex (\mathbb{C})

Hardware has **limited** approximations to them

Software extends **hardware** in many ways

Principles are largely language-independent

Apply to **Python, Perl, Java, Excel, Matlab, C, . . .**

. . . C++, Fortran, R, C#, Maple, Mathematica etc.

But mathematics and computing don't match

Not **just floating-point**, nor even **just hardware**

DON'T PANIC

Course will give a map through the minefield

With **moderate** care, can avoid **most** problems
Course helps to recognise dangerous areas

May help to debug when things do go wrong
Knowing that something **may** happen is key

- Some problems you can only watch out for
Will give guidelines on how to do that

Beyond the Course

Arithmetic/

Follow the link for further information /break

<http://www.cl.cam.ac.uk/teaching/1011/FPComp/>

There is some further reading in both of those

A few reasons are available – optional

Numerical Coding Book

Real Computing Made Real:
Preventing Errors in Scientific and
Engineering Calculations

by Foreman S. Acton

Good, clear book on avoiding **precision** loss etc.
Explains only how to prevent **some** forms of error!

Doesn't overlap with this course much

Consistency/Sanity Checking (1)

- Put in **lots** of this, **kept simple**

E.g. check values are valid and realistic

- Pref. every **entry/exit** of major code unit

Check most data being **used/returned/changed**

- No need to check everything, everywhere

Aim is to detect failures **early and locally**

```
if (speed < 0.0 .or. speed > 3.0e8) &  
    call panic("Speed error in my_function")
```

Consistency/Sanity Checking (2)

Ideally, something like:

```
def prevaricate (delay, reason) :  
    check_delay(delay)  
    check_reason(reason)  
    . . .  
    excuse = . . .  
    check_reason(excuse)  
    return excuse
```

Consistency/Sanity Checking (3)

- Write **sanity checker** for major data structures
Easy to add checking calls for debugging

call `sanity_upper (n, a, lda)`

call `sanity_rect (n, nrhs, b, ldb)`

call `dposv ('u', n, nrhs, a, lda, b, ldb, info)`

call `sanity_upper (n, a, lda)`

call `sanity_rect (n, nrhs, b, ldb)`

$O(n^3)$ calculation – $O(n^2)$ checking cost

Benefits of Checking

May **double** time taken to get code to compile
AND **halve** total time until it mostly works!

- Not restricted to numerical aspects
An old “**software engineering**” technique
Predates that term by many decades . . .

Won't cover any more of this here, but see
Debugging/

Using Classes

Don't be afraid to write your own **class**

You don't need to use any more memory

Modern compilers will compile that efficiently

- You can then check the values **systematically**

Especially useful for arithmetics like **complex**

Could check just multiplication and slower actions

- Don't forget to **initialise** on creation

Where Do Problems Arise?

Paradoxically, often for **integer** arithmetic!
People get careless with simple aspects

Real (i.e. **floating-point**) is a lot trickier
Most people are aware of that, in theory

- But it isn't as tricky as often thought
60 years of **Fortran** use shows that one!

Complex is a little trickier, but not much

Integers

- Mostly trivial, and just work as you expect
This course skips all of the simple aspects
Only **three** areas cause significant trouble

- Almost all problems arise with **overflow**

- Followed by **signed/unsigned** problems
This affects only **some** (**C**-like) languages

- Followed by the **division/remainder** rules

Will mention a **few** advanced features, as well

Division/Remainder Rules

If both M and N are positive, M/N rounds **down**
And $(M/N)*N + \text{remainder}(M,N) = M$

- **Language-dependent** if either are **negative**
Check its **specification** if you depend on that
Alternatively write a **run-time test**, and fix up

And, of course, **division by zero** is an **error**
Consequently, so is **remainder by zero**

That's all . . .

Unlimited Size Integers

- No limit on size, except **memory** and **time**

Built-in to **Python**, **BigInt** in **Perl**

Libraries (e.g. **GMP**) for **C**, **C++**, (**Java**, **Fortran?**)

Also **Mathematica**, **Maple**, **bc** etc.

Good packages are easy to use

- Eliminates overflow complexities
- But indefinite growth will crash program

And, only if you use **very** big numbers:

multiply/divide/remainder/conversion slow

Current Integer Hardware

Binary, twos' complement, e.g. for 8 bits:

$$01010011 = 2^6 + 2^4 + 2^1 + 2^0 = 83$$

$$11000101 = -2^7 + 2^6 + 2^2 + 2^0 = -59$$

16, 32 and 64 bits, rarely 8 and 128 bits

Overflow wraps: $2*83 = -90$ and $4*83 = 76$

- Your CODE may not wrap – see later

⇒ Means that $(M*N)/N$ may not be M

And other, similar, invariants may fail

Problems with Wrapping

parameter ($n = 1800$)
double precision $d(n,n,n)$
call $\text{init}(d, n*n*n)$

Assume 64-bit system with 32-bit integers

Very common environment nowadays

Equivalent to calling $\text{init}(d, 1537032704)$ – Oops!

- Can't avoid, so must watch out for it – how?

Checking for Wrapping

Either of the following will detect it

- Both cost very little in effort or time

```
ntotal = n*n*n
```

```
if (ntotal /= n*dble(n)*n) call panic(...)
```

```
ntotal = n*n*n
```

```
if ((ntotal/n)/n /= n) call panic(...)
```

- Even checking for negative bounds helps
Will pick up **over half** of such cases!

Integer Overflow (1)

Some **always use** floating-point (**Excel, Matlab**)

May **convert to** floating-point (**Perl, R**)

Convert to **unlimited** size (**Python** but **not numpy**)

Very rarely, trap it and diagnose the failure

- All **fairly** safe options for most use

May wrap modulo $|2^{bits}|$ (**Java, C#, numpy**)

- Generally **NOT** what you want (see later)

May be **UNDEFINED** (**C, C++, Fortran**)

Integer Overflow (2)

Be warned: wrapping modulo $|2^{bits}|$ is **dangerous**
Any **optimisation** can cause truly horrible effects
Even with none, there are some very nasty **gotchas**

- Sometimes option to **trap it**, diagnose and **stop**
NAG Fortran always does, **gfortran -ftrapv** enables it
gcc -ftrapv and **g++ -ftrapv** will trap **some** overflows
- Using **C# checked** keyword raises an **exception**
- These are the **best** solutions, when available

Undefined Behaviour

Major cause of wrong answers, crashes etc.

- Effects are **almost always unpredictable**
- Even **unrelated** differences may have effects
- Sometimes **debuggers** misbehave or crash
- Simple tests are **usually** misleading
- **Most** books / Web pages are misleading

Undefined behaviour \neq system dependence

Reasons are beyond this course – please ask

Over-Simplified Example

B = C = D = 5000

A = B*C*D = 445948416 Wrong

E = A/D = 89189 Wrong

print E 89189 Wrong but consistent

Fairly often actually compiles vaguely like:

A = B*C*D = 445948416 Wrong

E = A/D = 89189 Wrong but consistent

print E \Rightarrow print B*C

print E 25000000 \Leftarrow But this is E!

Integer Formatted I/O

- Representation not usually important
Most people never need to know it

Can read or display in any base:

Bin. **01010011** = dec. **83** = oct. **133** = hex. **A3**

May be explicit: **2r01010011** or **0xa3**

Most formatted I/O is done in decimal, anyway!

Unix may use **octal** – what is **136**? Or **0136**?

Using Integers as Bits

You can treat **integers** as **arrays of bits**

But not in **Matlab** or **R**, for good reasons

Bitwise **AND**, **OR**, **NOT** etc. make sense

Can even mix **bitwise** and **arithmetic** operations

All well-defined, portable and reliable

- **Except** for negative numbers

Keep all numbers **non-negative** and **in-range**

Negative numbers are for language lawyers

Shifting

Shift of N is multiply/divide by 2^N

- Don't shift negatives or **through** sign bit
It **may** work, but each language differs

- Keep all shifts **below** number of bits in word
Python is a rare exception to this

See the extra foils for why – it's bonkers!
A relic of **1950s** electronic constraints

Unsigned Integers

Mainly for C, C++, (& Java, Perl) users

Arithmetic modulo 2^{bits} (not $\text{GF}(2^N)$)

In 8 bits, $11000101 = 2^7 + 2^6 + 2^2 + 2^0 = 197$

As for hardware, numbers wrap round at 2^N

Numbers are always non-negative – e.g. $3-5 > 0$

- Divide/remainder aren't modular
- Pure unsigned arithmetic is fairly safe

Mixing Signed and Unsigned

- Signed/unsigned interactions are **foul**
Conversions are usually not what you expect
- It's very tricky to avoid mixtures in **C/C++**
Another **C/C++** warning – **char** may be either
More details for **C/C++** in extra information
- A minefield in all languages that have it
C/C++ people need to watch out for '**gotchas**'

Fixed-Point Arithmetic

Fixed number of digits after decimal point

Precision is part of variable's type

Usually implemented as scaled integers

Heavily used for financial calculations

Rare in scientific computing, but in bc/dc etc.

Generally easy to use, except for:

- Rounding of multiplication/division
- Mixing precisions, conversion, etc.
- Special functions (sqrt/log/etc.)

Scaled Fixed-Point

Fixed-point with a separate scale factor

Common in 1950s – replaced by true floating-point

C# decimal has resuscitated it

Possibly using IEEE 754 decimal floating-point

- Almost always, it's a complete waste of effort

True fixed-point or floating-point are better

It's closely related to unnormalised floating-point

Also a proposed DEC64 format (not covered further)

Rational Arithmetic

One of the main modes in **Mathematica**
Combined with **unlimited size integers**

Only serious problem is explosion of size
Otherwise, it works just as you would expect

Fixed size rationals have their advantages
Sometimes called **fixed-slash** arithmetic
Really esoteric – ask offline if interested

Basics of Floating-Point

Also called (leading zero) scientific notation

$sign \times mantissa \times base^{exponent}$

E.g. $+0.12345 \times 10^2 = 12.345$

$1 > mantissa \geq 1/base$ (“normalised”)

P sig. digits \Rightarrow relative acc. $\times (1 \pm base^{1-P})$

Also $-\maxexp < exponent < \maxexp$ – roughly

Like fixed-point $-1.0 < sign/mantissa < +1.0$

Scaled by $base^{exponent}$ (10^2 in above example)

Floating-Point versus Reals

- Floating-point effectively **not deterministic**
Predictable only to representation accuracy
Differences are either trivial – $\times (1 \pm base^{1-P})$
Or only for **infinitesimally small** numbers
 - **Fixed-point** breaks many rules of arithmetic
 - **Floating-point** breaks even more
- Wrong assumptions cause wrong answers**
- The key is to think **floating-point**, not **real**
Practice makes this semi-automatic

Invariants (1)

- Both are **commutative**:

$$A+B = B+A, \quad A*B = B*A$$

- Both have **zero**, **unity** and **negation**:

$$A+0.0 = A, \quad A*0.0 = 0.0, \quad A*1.0 = A$$

Each A has a $B = -A$, such that $A+B = 0.0$

- Both are **fully ordered**:

$A \geq B$ and $B \geq C$ means that $A \geq C$

$A \geq B$ is equivalent to NOT $B > A$

Invariants (2)

The following are **approximately** true
Don't assume that they are **exactly** true

- Neither **associative** nor **distributive**:
 $(A+B)+C$ may not be $A+(B+C)$ (ditto for $*$)
 $(A+B)-B$ may not be A (ditto for $*$ and $/$)
 $A+A+A$ may not be $3.0*A$

Invariants (3)

- They do not have a **multiplicative inverse**:
Not all A have a $B = 1.0/A$, such that $A*B = 1.0$
- Not **continuous** (for any of $+$, $-$, $*$ or $/$):
 $B > 0.0$ may not mean $A+B > A$
 $A > B$ and $C > D$ may not mean $A+C > B+D$
 $A > 0.0$ may not mean $A > 0.5*A > 0.0$

Remember School Maths?

Above is true for **all fixed-size floating-point**
Whether on a computer or by hand in decimal

- But were you taught that at school?

It doesn't cause too much trouble
But it **does** take some getting used to

Current Floating-Point Hardware

IEEE 754 a.k.a. IEEE 854 a.k.a. ISO/IEC 10559

<http://754r.ucbtest.org/standards/754.pdf>

Binary, signed magnitude – details are messy

- 32-bit = 4 byte = single precision

Accuracy is 1.2×10^{-7} (23 bits),

Range is 1.2×10^{-38} to 3.4×10^{38}

- 64-bit = 8 byte = double precision

Accuracy is 2.2×10^{-16} (52 bits),

Range is 2.2×10^{-308} to 1.8×10^{308}

Other Sizes of Floating-Point

- Don't go there – ask if you might need to
IEEE 754 dominates people's thinking

May have **128-bit IEEE 754R** floating-point

In several different variations . . .

It may be **very much** slower than **64-bit**

Exact FP arithmetic usually futile (explosion)

Interval arithmetic trendy but little better

Arbitrary precision is easy, but out of fashion
but **Mathematica** has it (almost unusably)

Intel/AMD Arithmetic

- Avoid it completely if you can
Generally becoming less used
Compilers/packages often use it **internally**
- One cause of differences in results

80-bit: accuracy is 1.1×10^{-19} (**63** bits),

Range is 3.4×10^{-4932} to 1.2×10^{4932}

Typically stored in **12** or **16** bytes (**96** or **128** bits)

<http://www.intel.com/design/...>

[.../pentium4/manuals/index_new.htm](http://www.intel.com/design/pentium4/manuals/index_new.htm)

Decimal Floating-Point (1)

Added to **IEEE 754R** at **IBM**'s instigation
Both **IBM** and **Intel** **were** going to put it in **hardware**
One **Python** module **emulates** it (in **software**)
It is beginning to look doubtful that it will take off

- It is **NOT** a panacea – **OR** any worse
Exactness claims (**Python** etc.) are propaganda
Try π , $1.0/3.0$, 1.01^{25} , scientific code

It is claimed to help emulate decimal **fixed-point**

- That is complete and utter hogwash
Scientific programmers aren't interested, anyway

Decimal Floating-Point (2)

In binary floating-point, if $a \leq b$:

$$a \leq a/2 + b/2 \leq b \quad \& \quad a \leq (a + b)/2 \leq b$$

But not necessarily in decimal floating-point

The other “gotchas” are extremely arcane

It may look more accurate, but it isn't

Writing portable code is easier than it appears

NAG was base-independent before **1990**

But **Intel** have dropped it and **IBM** has backed off

- Will it ever be relevant to **scientists**? Probably **not**

Denormalised Numbers

- Only in **IEEE 754** systems, and not always
Minimum exponent and zeroes after point
E.g., in decimal, 0.00123×10^{-308}
- Regard numbers like that as mere noise
- Replaced by **zero** if too small (**underflow**)
Never trapped nowadays – codes fail if it is
- Numeric advantages **and** disadvantages
Can be **very slow** – may take **interrupt**
Often **option** to always replace by **zero**

Denorms and Underflow

- Not generally a major problem

Use **double precision** to minimise traps

Almost always safe to replace by zero

$(A/2.0)*2.0$ may not be A

$A > 0.0$ does not mean $2.0*A > 1.5*A$

$B > C$ does not mean $B-C > 0.0$

And many others . . .

- **Hard underflow** code mishandles **denorms**

See later about **binary I/O**

Error Handling and Exceptions

Here be dragons ...

The following is what you **NEED** to know
Most of the details have been omitted
Will return to a few aspects later

- **PLEASE** contact me if you hit a problem

Other Exceptional Values

Zeroes are signed – but try to ignore that

- \pm infinity represents value that overflowed
Not necessarily large – e.g. $\log(\exp(1000.0))$
- NaN (Not-a-Number) represents an error
Typically mathematically invalid calculation

In theory, both propagate appropriately

- In practice, the values are not reliable

What Can Be Done?

Consistency/sanity checking – **yes, Yes, YES!**

- **Double precision** reduces overflow problems
Can run **faster**, by avoiding **exceptions/denorms**
- Don't assume **first catch** is **first failure**
- Don't assume **no catches** means **no failures**

The above rules apply to most classes of error
E.g. array bound overflow, pointer problems

Floating-Point Overflow

Mathematica uses a fancy format and rarely overflows

Excel delivers “NUM!”

NAG Fortran always traps overflow

Some other compilers have a trapping option

All others deliver an infinity of right sign

numpy default gives a warning but not an exception

In itself, that would be perfectly reasonable and safe

I.e. it's just using the affine extension of the reals

⇒ But remember the optimisation problems!

Divide by Zero etc.

Python, Perl, Excel, Matlab, Mathematica trap $A/0.0$
C, C++, Fortran rarely do (except for NAG)
Java, R, C# don't treat it as an error!

⇒ If not, divide-by-zero also gives infinity

numpy behaves exactly as for overflow

The sign of the infinity depends on the sign of zero
This is claimed to be “meaningful” – ha, ha!

Infinitities and Errors

If we have $B = A - A$; $C = -B$; $D = C + 0.0$;

All of $B = C = D = 0.0$

But $1.0/B \neq 1.0/C$ and $1.0/C \neq 1.0/D$

- \Rightarrow Don't trust the sign of infinities
 - If you can, trap errors, diagnose and stop
- In IEEE 754 terms, the serious errors are:
Overflow, divide by zero and invalid

Trapping

NAG Fortran always traps arithmetic errors

With gfortran/gcc/g++, use
-ffpe-trap=invalid,zero,overflow

With Intel (ifort/icc/icpc), use -fpe0

With numpy use:

seterr(over='raise',divide='raise',invalid='raise')

Or can use 'call' rather than 'raise'

Advanced Example

```
program fred
  double precision :: x = -1.0d-300
  do k = 1,6
    x = x-0.9d0*x
    print *, 1.0d0/x
  end do
end program fred
```

```
-1.0E+301
-1.0E+302
. . .
-1.0E+308
-Infinity
. . .
-Infinity
+Infinity
+Infinity
```

Signs of Zero and NaN

The same applies to functions that test signs

- Functions like **Fortran SIGN**, **C copysign**
And many others in **C99** and followers

The signs of **zeros** and **NaNs** are interpreted
Never mind that those signs are meaningless

- Regard the result as an **unpredictable** value
See the extra information for more details

NaNs and Error Handling

Invalid operations **may** result in a NaN

$0.0/0.0 = \text{infinity}/\text{infinity} = \text{infinity}-\text{infinity} = \text{NaN}$

Operations on NaNs **usually** return NaNs

- But NaN state is very easy to lose
C99, Java actually **REQUIRE** it to be lost

Few examples of **MANY** traps for the unwary

$\text{int}(\text{NaN})$ is often 0, quietly

$\text{max}(\text{NaN}, 1.23)$ is often 1.23

Comparisons on NaNs usually deliver **false**

Sanity Checking and NaNs

if $x \neq x$ then we have a NaN – in theory
In practice, may get optimised out

But don't make all tests positive checks
First example in course would be better as:

```
if (speed > 0.0 .and. speed < 3.0e8) then
    continue
else
    call panic('Speed error in my_function')
endif
```

Complex Numbers

- Generally simple to use (but C99's aren't)
Always (real,imaginary) pairs of FP ones
Python, Fortran, C++, Matlab, R, C99 (sort of)
Optional package for Perl, Java
Fortran usually most efficient for them

I/O usually done on raw FP numbers

- Easy to lose imaginary part by accident
Special functions can be slow and unreliable
- Don't trust exception handling an inch
It will often give wrong answers, quietly
Reasons are fundamental and mathematical

Mixed Type Expressions

Integer \Rightarrow float \Rightarrow complex usually OK

N-bit integer \Rightarrow N-bit float may round weirdly

Float \Rightarrow integer truncates towards zero

Complex \Rightarrow float is real part

- You **won't** generally get any **warning**

Overflow is **undefined** in **C** , **C++** , **Fortran**

Java is defined, but **very dangerous**

Other languages are **somewhat** better

- **Infinites** and **NaNs** are **Bad News**

Complex and Infinities or NaNs

- This is a disaster area, to put it mildly
Don't mix **complex** with **infinities** or **NaNs**
All such code is effectively **undefined**

- That means **float** \Rightarrow **complex**, too
If the former has any of the **exceptional values**

See the extra information for some sordid reasons

- Regard complex overflow as **pure poison**
Put in your own checks to stop it occurring

Other Arithmetics

Let's use **Hamiltonian Quaternions** as an example

- Not going to cover them in this course!

Very few languages have them **built-in**

Can get **add-on packages** for most languages

Type extension can make look like **built-in types**

- Almost **no extra problems** over complex numbers

Main difference is that are **not commutative**

Other **advanced arithmetics** are similar

For example, true **Galois fields** and so on

Formatted Output

Generally safe (including `number` \Rightarrow `string`)

- Accuracy of `very` large/small may be poor

- Values like `0.1` are not exact in binary

Decimal `0.1` = binary `0.0001100110011001...`

Only `6/15` sig. figs guaranteed correct

But need `9/18` sig. figs for guaranteed re-input

- Check on `infinities`, `NaNs`, `denorms`

If implementation is poor, will fail with those

Formatted Input

Far more of a problem than output

- Overflow and errors often **undefined**

Often doesn't detect either or handle sanely

Behaviour can be very weird indeed

Infinities, NaNs, denorms are always unreliable

Don't trust the implementation without checking

- Always do a minimal cross-check yourself

Undefined Behaviour and I/O

Generally, I/O conversion is predictable

- But only for one version of one compiler

But does mean that you can rely on tests

Actual conversion is in library, not code

All sharing compilers may behave the same way

Any upgrade may change behaviour

- It's worth preserving and rerunning tests

Binary (Unformatted) I/O

Shoves internal format to file and back again

Fast, easy and preserves value precisely

- Don't use **between systems** without testing

- Depends on **compiler, options, application**

Different languages use different methods

Solutions exist for **Fortran** \Leftrightarrow **C**

Derived/fancy types may add extra problems

- Can give almost complete checklist

Checklist for Binary I/O

- Must use **same sizes, formats, endianness**
Sizes are 32/64-bit mode, precision etc.

Formats are primarily application or language
Basic data types use the **hardware formats**
Derived types depend on the compiler etc.

“**Little endian**”: **Intel/AMD, Alpha**

“**Big endian**”: **SPARC, MIPS, PA-RISC, PowerPC**

Either: Itanium **Mixed: dead?**

May be compiler/application conversion options

Cross-Application Issues

Most compilers & applications are compatible

Cross-system transfer can be tricky

All systems now use very similar conventions

- But there are occasional exceptions
Especially with **Fortran unformatted** I/O

You probably won't hit problems with this

If you do, ask for help – it's not a big problem

IEEE 754 Issues

May be problems with **denorms**, **infinities**, **NaNs**
Can be chaos if code can't handle them

- Easy to write a simple test program
Just write an unformatted file with them in
Read it in, and check that they seem to work

0.0, **$\pm 10^k$** ($k = -323 \dots + 308$), **$\pm \text{inf}$** , **NaN**
Compare, **add**, **subtract**, **multiply** and **divide**
on all pairs – c. 8 million combinations
Crudely, print **12** digs, and use **diff**

Single Precision (32-bit)

- Do **NOT** use this for serious calculations
Cancellation / error accumulation / conditioning
Much more likely to trip across exceptions

$x^2 + 10^4 \times x + 1$ roots are c. 10000 and 0.001

$(-b \pm \sqrt{b^2 - 4ac}) / (2a)$ in 32-bit

Delivers c. 10000 and true zero – oops!

- Lots of memory allows for big problems
Even stable big problems need more accuracy
 1.2×10^{-7} often multiplied by matrix dimension

GPU Issues

Single precision is a lot faster than double

- You may need to use it for performance
- Some problems are very stable – no problem

But, in general, this is a major headache

- First check for a more stable algorithm
- There are precision–extension techniques
Commonly used 30+ years ago, now needed again
Ask your supervisor to contact me if it might help

Numerical Analysis (1)

Analyses effects of approximate calculations

Not covered here – DAMTP has 3 courses on it

Recommended to use a package or library:

- NAG library is most general reliable library
- Good open-source libraries (e.g. LAPACK)
- Many others are seriously unreliable or worse
- Do NOT trust Numerical Recipes or the Web

Arithmetic/

Numerical Analysis (2)

Many good, often old, **numerical analysis** books
Many are hard going and expensive or out-of-print
Following is good, affordable and available

**Numerical Methods That Work: an Introduction
to Numerical Techniques and Problems**
by **Foreman S. Acton**

Problem is it really **IS** an introduction
And, even then, it's not exactly bedtime reading!

Accuracy and Instability

Results almost never better than input (**GIGO**)

- Do **NOT** assume machine precision in result

Errors can often build-up exponentially

Single \Rightarrow **double** may not help

- In that case, must improve algorithm

Trivial (not very realistic) example:

K 'th differences of x^K , $x=0.5, 0.51, \dots, 1.99, 2.0$

In D.P., 1 sig. fig. at $K=7$, nonsense thereafter

Cancellation (1)

- Low-level cause of most loss of accuracy
Caused by subtracting two nearly-equal values

Obviously, includes adding two with different signs

- But also dividing (and multiplying by inverse)

Assume numbers have P digits of precision

X and Y have Q leading digits in common

$\Rightarrow X - Y$ and $X/Y - 1.0$ have precision $P - Q$

- Restructuring expressions can help a lot

Cancellation (2)

Where it matters, consider changes like the following:

$$(X+D)**2-X**2 \Rightarrow (2*X+D)*D$$

$$x^5-y^5 \Rightarrow (x^4+x^3*y+x^2*y^2+x*y^3+y^4)*(x-y)$$

$$\sin(x+d)-\sin(x) \Rightarrow \sin(x)*(\cos(d)-1.0)+\cos(x)*\sin(d)$$

I haven't used this, but you might like to try:

<http://herbie.uwplse.org/>

Cancellation (3)

- Watch out for **large summations**, too

Look up **Kahan summation** for a better method

I use another, or emulate extended precision:

C++/...

.../Exercises/Chapter_24/fancy_accumulate.cpp

.../Exercises/Chapter_24/fancy_inner.cpp

Unfortunately, it may be **implicit** in the **algorithm**

Common with ones that use **numerical derivatives**

Realistic Cases of Problem

Linear equations, determinants, eigensystems
Solution of polynomials, regression, anova
ODEs, PDEs, finite elements etc.

- Any method works in **simple, small** cases
Poor ones fail in **complex, larger** ones
- Put **consistency checks** in your program
- Use **high-quality** algorithms and libraries
- Try **perturbing** your input and check effects
- As always, find out what the **experts** advise

Topics Not Covered (1)

The details of any of the above topics
Too many other topics to list

Examples of areas that could have courses:

Parameterisation in C, C++, Fortran etc.

Interval arithmetic and its uses

Introduction to numerical analysis

C99 and its consequences

Topics Not Covered (2)

Older or rarer systems/problems/issues
Number handling in external protocols
Model, use and analysis of **IEEE 754**
IEEE 754R and decimal floating-point
Interactions with operating systems
Implementation techniques and implications
Mathematical models of computer arithmetic
And so on . . .

Reminder – Trapping Options

NAG Fortran traps everything by default

For gfortran/gcc/g++ use
-ftrapv -ffpe-trap=invalid,zero,overflow

For Intel (ifort/icc/icpc), use -fpe0

For Python numpy use
seterr(over='raise',divide='raise',invalid='raise')

For C# use checked keyword or option