Numerical Tools for Physical Scientists

Feb/Mar 2013

The Course

- We've covered some basics of programming for scientists in the last class:
  - C/C++
  - git for version control
  - unit tests
- Here we're going to focus on specifics of numerical computing for physical scientists.

Course Outline

- Today: Intro, Numerics
- Feb 14: Random Numbers
- Feb 26: Integration, ODE solvers
- Feb 28: Molecular Dynamics
- Mar 5: Numerical Linear Algebra I
- Mar 7: Numerical Linear Algebra II, PDEs
- Mar 12: Fast Fourier Transforms I
- Mar 14: Fast Fourier Transforms II

Today

- What numerical computing is, and how to think about it
- Modelling vs reality; Validation & Verification
- Real arithmetic on computers - floating point math
- Random Number Generators

Computational Science

- "Third Leg" of Science?
- Different than theoretical science or experimental science; requires skills of each
- "Experimental theory" - exploring complex regions of theory
- Requires note-taking, methodical approach of experimentalists; mathematical chops of theorists; and other knowledge too.

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Computational Science

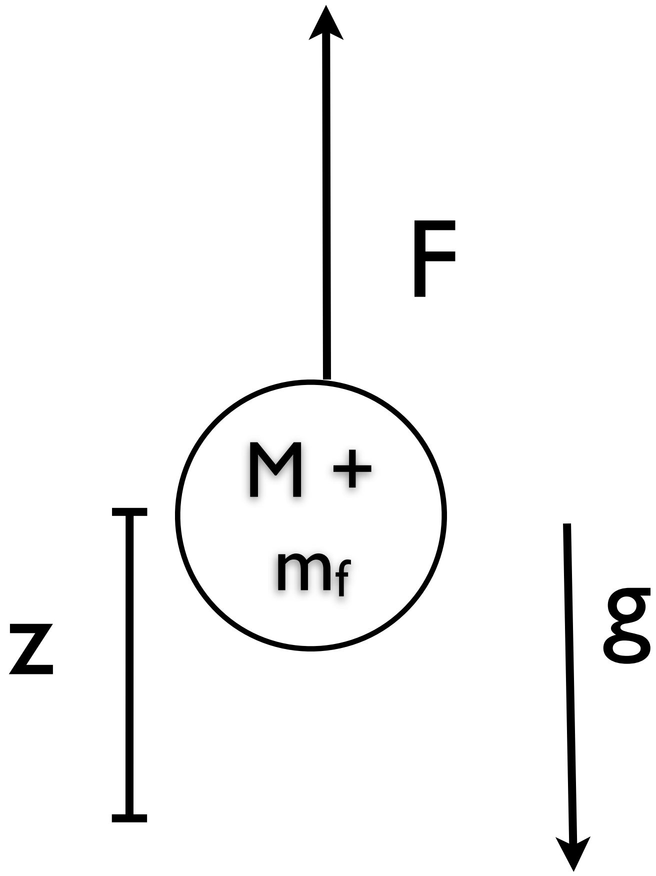
- Often done incredibly badly
- If experimentalists work was of quality of much computational work, we still would be arguing over the charge on an electron
- Experimentalists, theoreticians have had centuries to determine best practices for their disciplines
- Computationalists starting to develop ours - eg this course.

Computational Science

- Computational science, like experimental or theoretical science, is a *modelling* endevor
- Creating simplified picture of reality that includes (only) bits you want to study.

Phenomenon

Conceptual/ Mathematical Model



$$\ddot{z} = m(t)(F - g)$$

$$\dot{m}_f \propto F$$

Numerical Computation

```
double dfdt(double time, double mass, double fuelmass,
            double vel, double force, double z, double dt,
            double *df) {

      double g = Mearth*newtonG/(z*z);

      df[0] = (mass+fuelmass)*(alpha*burnrate-g);
      df[1] = vel;
      df[2] = burnrate;

}
~
~
                                        1,1           All
```

Phenomenon

model

Conceptual/
Mathematical Model

model

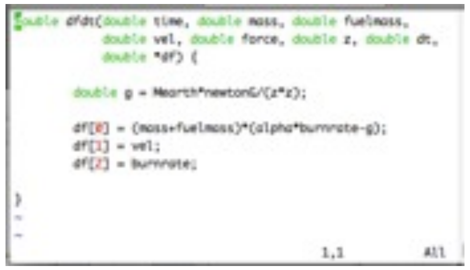
Numerical
Computation

Can go wrong at each step

Are we solving the right equations?

$$\ddot{z} = m(t)(F-g)$$

$$\dot{m}_f \propto F$$



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Can go wrong at each step

$$\ddot{z} = m(t)(F - g)$$

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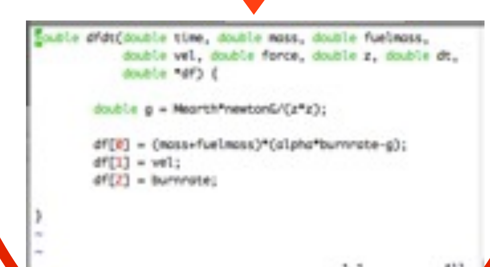

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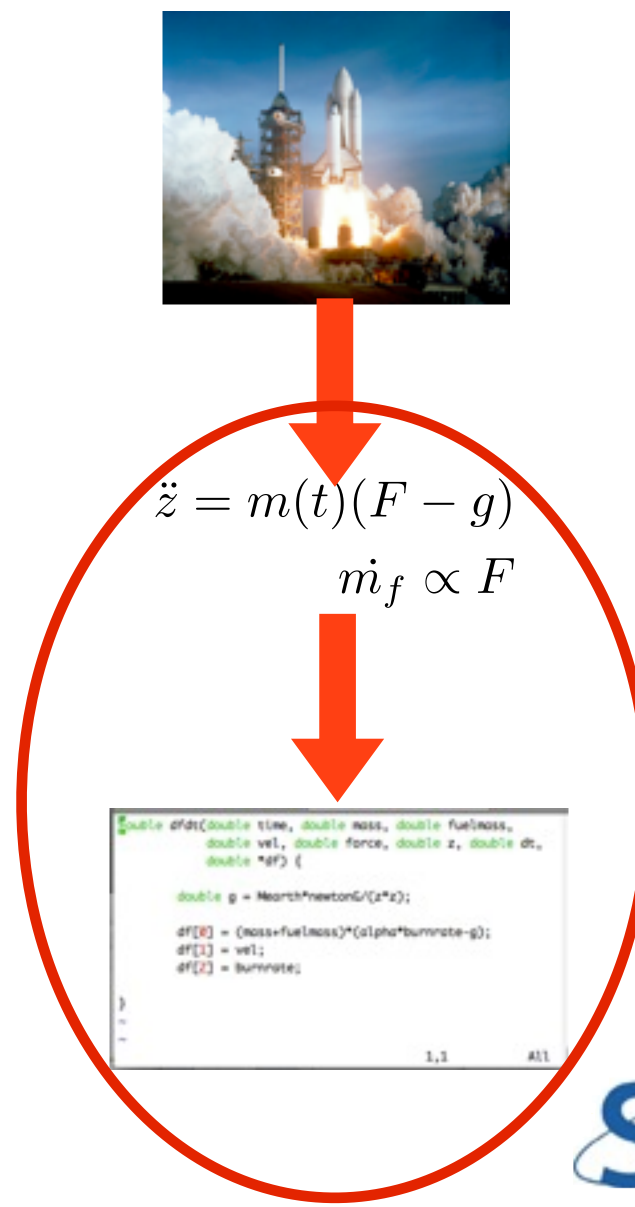
}
```

Verification: Testing math ⇒ numerics

- Can go wrong in translation from mathematical model to computational model

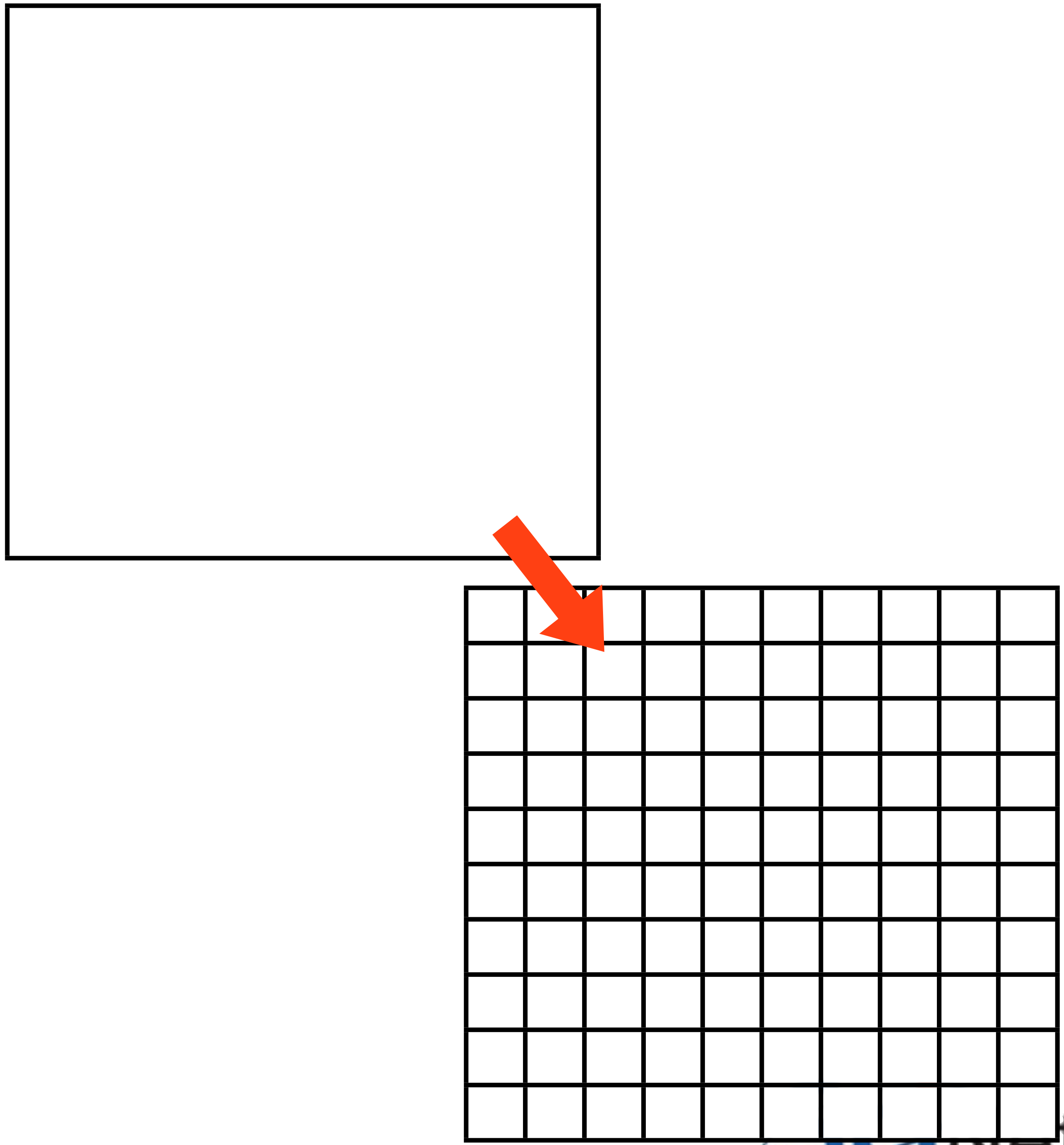
- Discretization error, Truncation error, roundoff, ... or just plain bug.

- Process of testing this: Verification



Discretization error

- Error caused by going from continuum to discrete domain
- Eg: grid in space; discrete timesteps; etc.
- Should decrease as you increase resolution.



Truncation Error

- Typically occurs when an expansion is truncated

$$e^x \approx 1 + x + \frac{x^2}{2}$$

Roundoff

- Floating point mathematics can go wrong (more on this later)

$$(a+b)+c \neq a+(b+c)$$

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Just plain bugs

- Scientific software can get large, complex
- Bugs creep in
- Unit testing, version control can greatly help
- Still happens

Verification: Analytics, Bechmarks, Comparisons

- Trying to make sure we are correctly solving the intended equations in the regime of interest.
- Comparison to known analytic solutions:
  - Easy to do
  - Solutions tend to be of very simple situations - not hard tests of the computation, particularly integrated.
  - But very useful for unit tests.

Verification: Analytics, Bechmarks, Convergence

- Trying to make sure we are correctly solving the intended equations in the regime of interest.

- Benchmarking a complex solution from your code to that of another code (could be: same code last year, saved results)

    - CAN NOT show that either solution is *correct*

    - CAN show that at least one code/version has a problem, or that something has caused changes.

Verification: Analytics, Bechmarks, Convergence

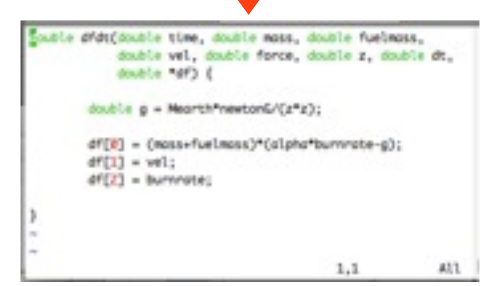
- Trying to make sure we are correctly solving the intended equations in the regime of interest.
- Convergence testing: compare solutions at higher and higher resolution (or terms in expansion, or...)
- Again, doesn't mean converges to correct result, but lack of convergence indicates a problem
- Relatedly - does slightly varying input parameters, result in robust result, or do huge changes occur in relevant metrics?

Validation: Testing reality ⇒ numerics

- Can go wrong in translation from phenomenon to mathematical model

$$\ddot{z} = m(t)(F - g)$$

$$\dot{m}_f \propto F$$



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    df[2] = burnrate;

}
```

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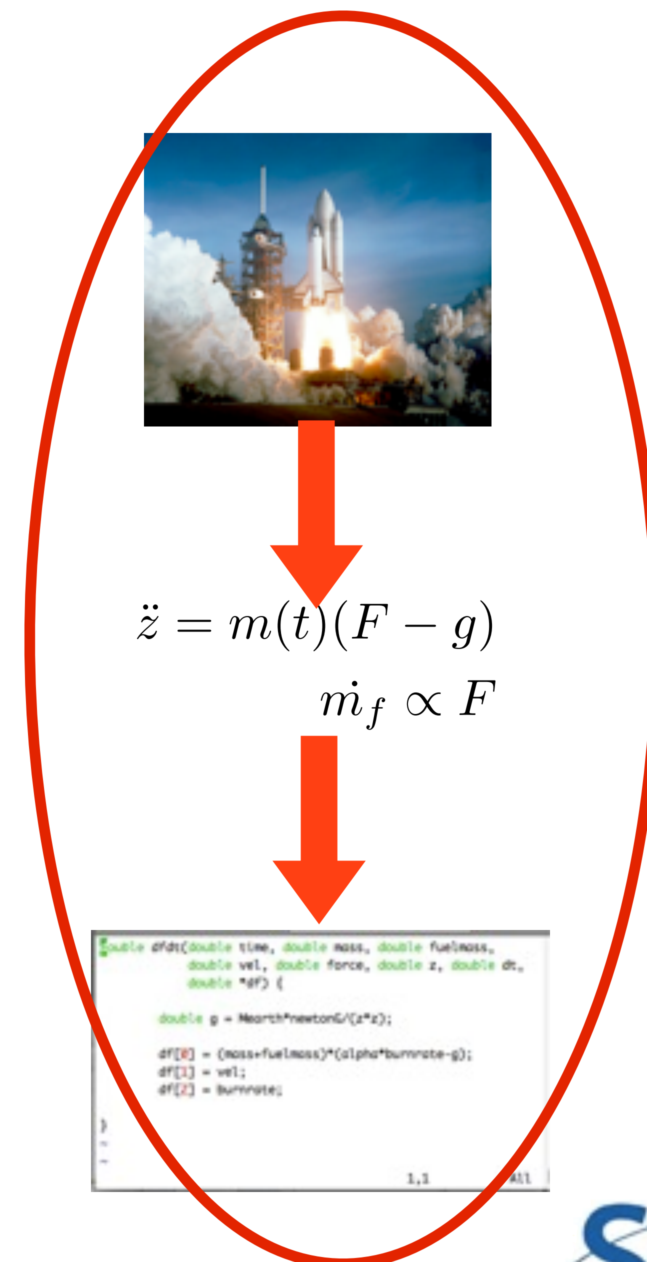
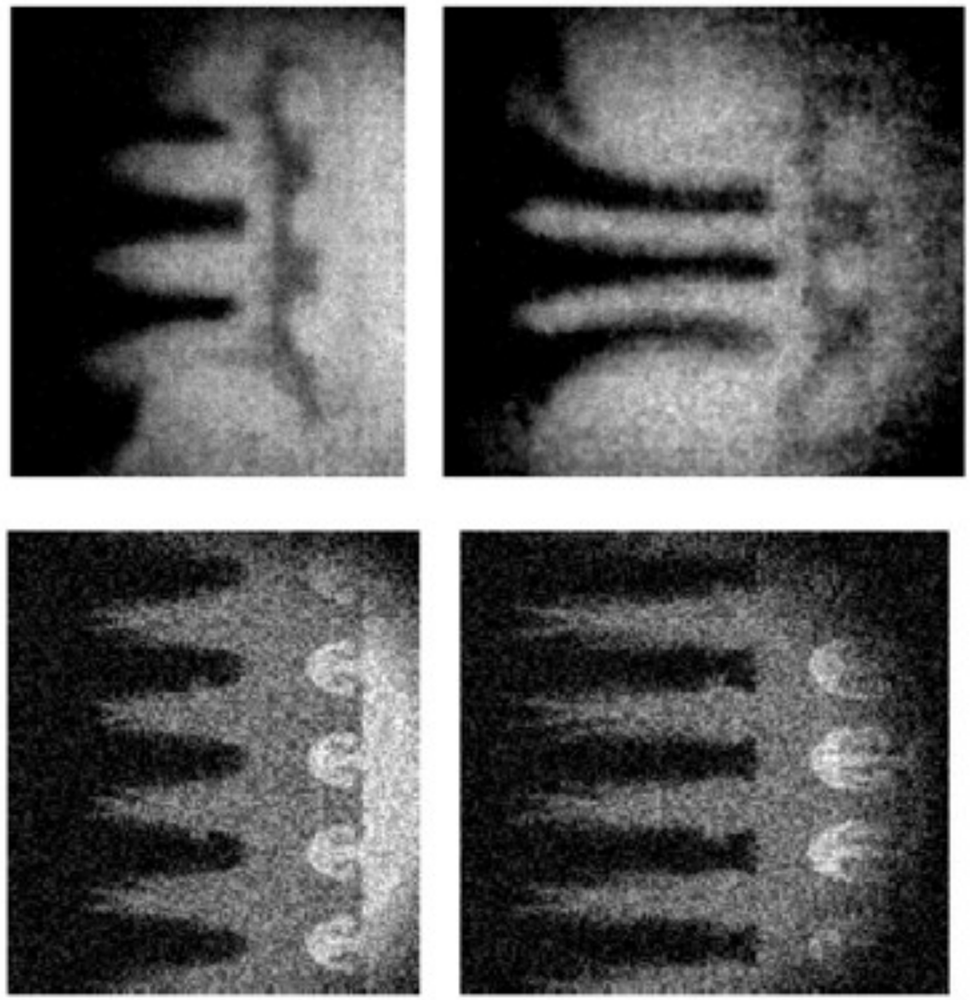
Validation: Testing reality ⇒ numerics

- Can go wrong in translation from phenomenon to mathematical model
- Typically only implementation of full mathematical model you have is the code
- Testing code against reality



Validation: Code/ Experiment comparisons

- Only way to do validation is to compare directly to experimental results
- Must be in regime you are realistically interested in, but still experimentally accessible
- Requires collaboration with experimentalists.
- Proves that there's a regime in which your code accurately reproduces reality.



arXiv:astro-ph/0206251

Not a one-off

- Even after an extensive V&V effort, code changes
- Still giving right answer?
- Unit tests, **regular** integrated tests crucial to *maintaining* correctness
- Who cares that your code once gave correct answer *once*, some Thursday two years ago?

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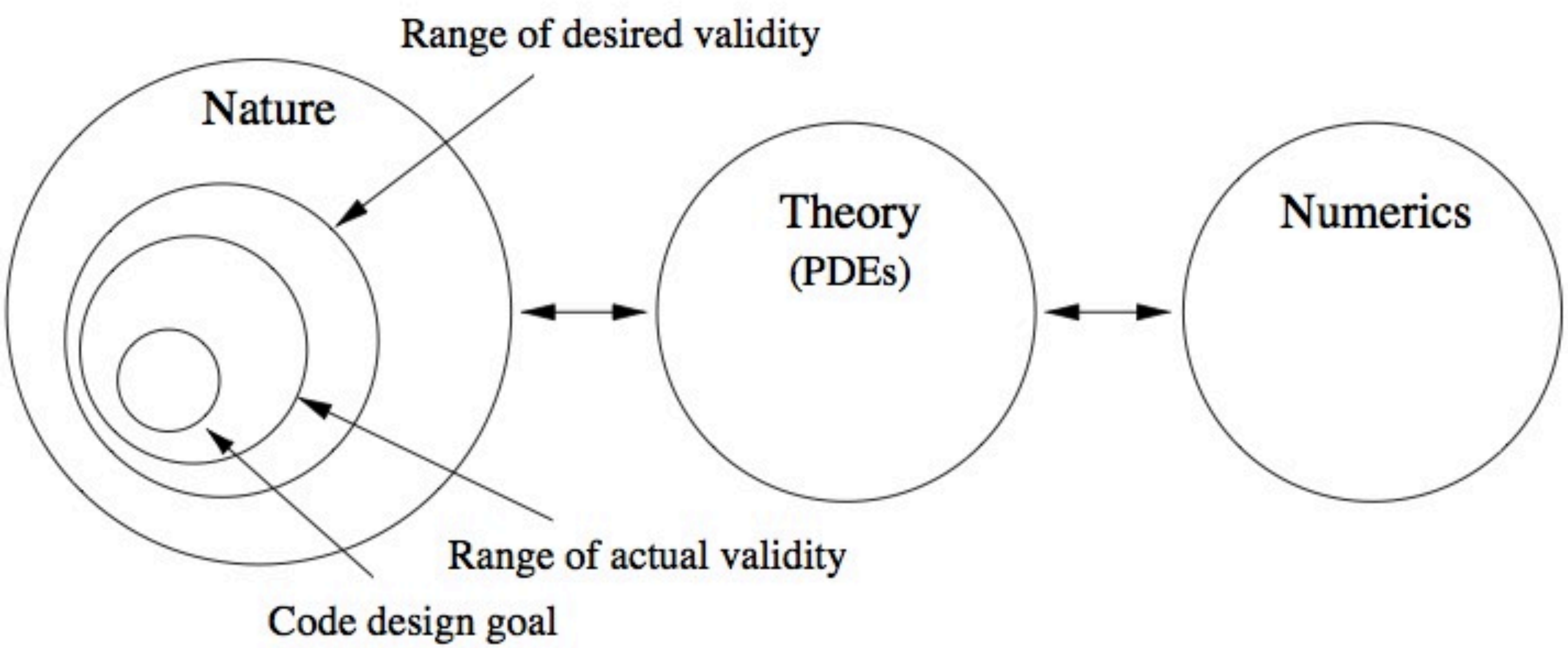
Regimes of Interest



Floating Point Mathematics

Like real numbers, but different.

Integer Math and Computers

- Infinite number of integers
- Finite size of integer representation
- Finite range. One bit for sign; can go from -2^{31} to (almost) 2^{+31} (−2,147,483,648 to 2,147,483,647)
- Unsigned: $0..2^{32}-1$

int: 32 bits = 4 bytes

Integer Math and Computers

- long long int:
- One bit for sign; can go from -2^{-63} to (almost) 2^{+63} (−9,223,372,036,854,775,808 to 9,223,372,036,854,775,807)
- Unsigned: $0..2^{64}-1$

long long int: 64 bits = 8 bytes

Integer Math and Computers

- All integers within range are exactly representable.
- Absolute spacing (1) constant across range; relative spacing varies
- All operations (+,-,*) between representable integers represented unless overflow (with either sign)

Fixed point numbers

- Could treat real numbers like integers - 0...INT_MAX, with say the last two digits ‘behind decimal point’.
- Financial stuff often uses this; only ever need/want two decimal points
- Horrifically bad for scientific computing - relative precision varies with magnitude; cannot represent small and large numbers at same time.

Floating Point Numbers

- Analog of numbers in scientific notation
- Inclusion of an exponent means point is “floating”
- Again, one bit dedicated to sign

$$\underbrace{-}_{\text{sign}}\underbrace{1.34}_{\text{mantissa}} \times \overset{\text{base}}{10}{}^{\underbrace{-7}_{\text{exponent}}}$$

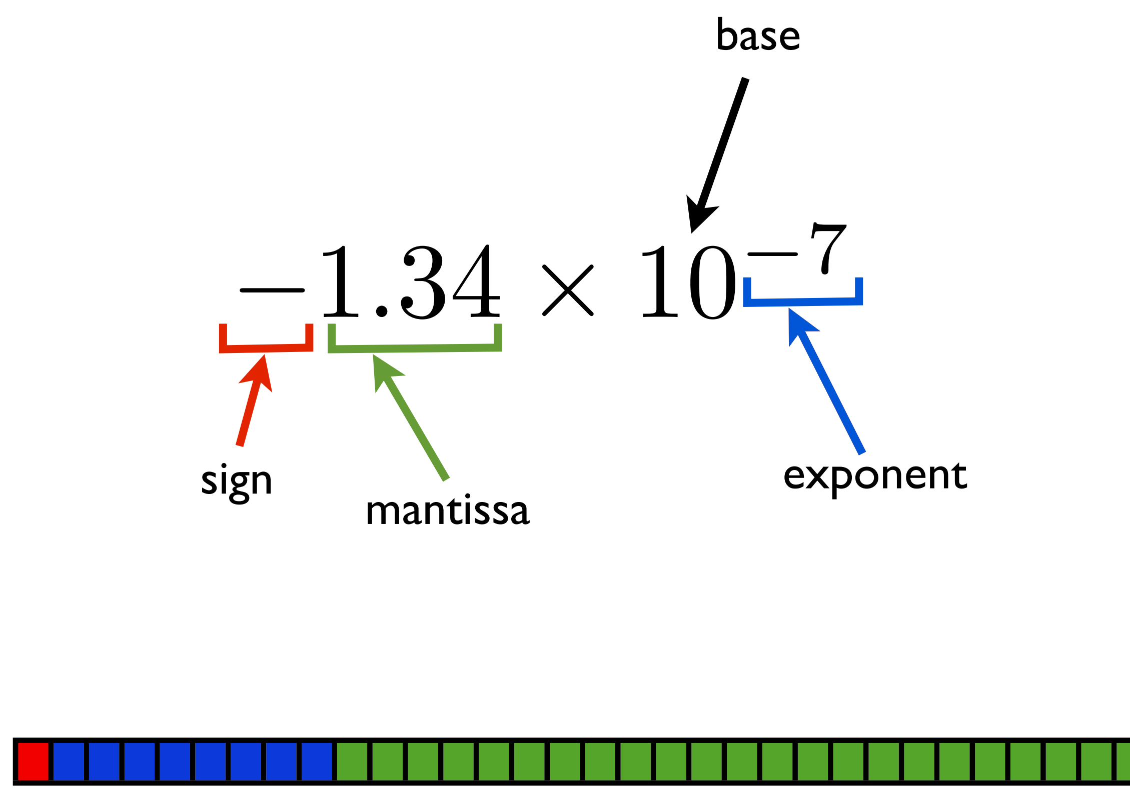
Floating Point Numbers

- **Standard**: IEEE 754
- Single precision real number (float):
- 1 bit sign
- 8 bit exponent (-126..127)
- 23 bit mantissa
- double precision: 1/11/52

$$\underbrace{-}_{\text{sign}}\underbrace{1.34}_{\text{mantissa}} \times \overbrace{10}^{\text{base}}{}^{\underbrace{-7}_{\text{exponent}}}$$

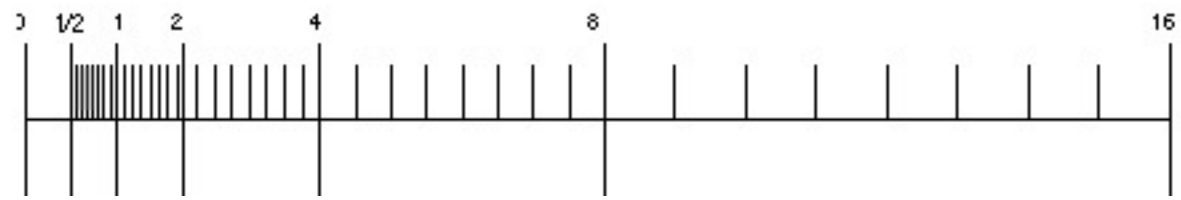
Floating Point Numbers

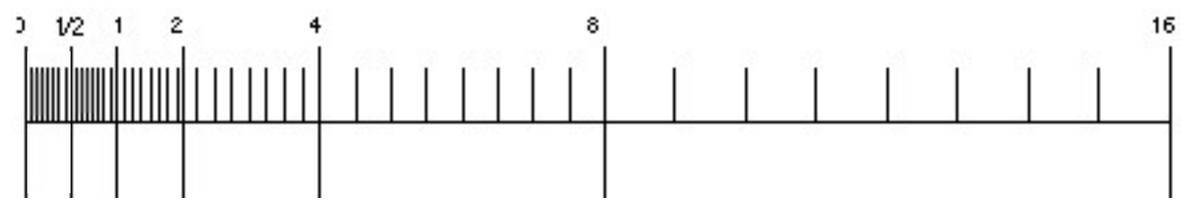
- To ensure uniqueness of represention (don't waste patterns), first bit of mantissa always 1.
- Since always 1, don't need to store it
- Really 24 (53) bits of mantissa
- Normalized numbers



Denormal numbers

- This actually leads to a big jump between smallest possible number and zero
- Relative accurracy doesn't degrade gracefully
- So *if* exponent = minimum, assume first bit of mantissa = 0





Special "Numbers"

- There's room in the format for the storing of a few special numbers:
- Signed infinities (+Inf, -Inf): result of overflow, or divide by zero.
- Signed zeros - signed underflow, or divide by +/-Inf
- Not a Number - NaN.   Sqrt of a negative, 0/0, Inf/Inf, etc.
- All of the events which lead to these are (usually) errors and can be made to cause exceptions.

Underflow: mostly harmless?

- Try the following:
- Repeatedly take sqrts, then square a number
- Plot this from 0..2
- What should you get? What do you get?
- Loss of precision in early stage of calcuation can cause problem

```
In [9]: def sqrts(x):
   ...:     y = x
   ...:     for i in xrange(128):
   ...:         y = sqrt(y)
   ...:     for i in xrange(128):
   ...:         y = y*y
   ...:     return y
   ...:

In [10]: x = linspace(0.,2.,1000)

In [11]: y = sqrts(x)

In [12]: plot(x,y,'o-')
```

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Floating Point Exceptions

- Let's look at the following Fortran code
- Second division should fail
- If compile and run as is, will just print NaN for C
- Can have it stop at error:

```
program nantest
    real :: a, b, c

    a = 1.
    b = 2.

    c = a/b
    print *, c,a,b

    a = 0.
    b = 0.

    c = a/b
    print *, c,a,b

    a = 2.
    b = 1.

    c = a/b
    print *,c,a,b
end program nantest
```

Floating Point Exceptions

- Compiling with gfortran, can give -ffpe-trap options
- will trap (throw exception, stop) for invalid, divide by zero, overflow
- Could also do underflow
- Debugger stops at line that causes exception

```
$ gfortran -o nantest nantest.f90
   -ffpe-trap=invalid,zero,overflow -g

$ gdb nantest
[...]
(gdb) run
Starting program: /scratch/ljdursi/Testing/fortran/na
  0.50000000       1.0000000       2.0000000

Program received signal SIGFPE, Arithmetic exception.
0x0000000000400384 in nantest () at nantest.f90:13
13            c = a/b
Current language:  auto; currently fortran
```

Floating Point Exceptions

- C: include fenv.h, and use feenableexcept (enable exceptions)
- constants defined
- gdb again works

```
#include <stdio.h>
#include <fenv.h>

int main(int argc, char **argv) {
    float a, b, c;
    feenableexcept(FE_DIVBYZERO | FE_INVALID | FE_OVERFLOW

    a = 1.;
    b = 2.;

    c = a/b;
    printf("%f %f %f\n", a, b, c);

    a = 0.;
    b = 0.;

    c = a/b;
    printf("%f %f %f\n", a, b, c);

    a = 2.;
    b = 1.;

    c = a/b;
    printf("%f %f %f\n", a, b, c);

    return 0;
}
```

Floating Point Exceptions

- C: include fenv.h, and use feenableexcept (enable exceptions)
- constants defined
- gdb again works

```
$ gcc -o nantest nantest.c -lm -g
$ gdb ./nantest
[...]
(gdb) run
Starting program: /scratch/s/scinet/ljdursi/Testing/
exception/nantest
1.000000 2.000000 0.500000

Program received signal SIGFPE, Arithmetic exception.
0x00000000004005d0 in main (argc=1, argv=0x7fffffffe4
nantest.c:17
17       c = a/b;
```

Floating Point Math

- Fire up Python, and try the following:

```
In [1]: print 1
1

In [2]: print 1.e-17
1e-17

In [3]: print (1. + 1.e-17) - 1.
??

In [4]: print (1. - 1.) + 1.e-17
??
```

Floating Point Math

- Fire up Python, and try the following:

```
In [1]: print 1
1

In [2]: print 1.e-17
1e-17

In [3]: print (1. + 1.e-17) - 1.
0.0
```

Errors in Floating Point Math

- Assigning a real to a flaotting point variable involves truncation
- Error of 1/2 ulp (Unit in Last Place) due to rounding due to assignment to finite precision
- (single precision: 1 part in 2^{-24} ~ 6e-8; double, 1e-16)

$$
\begin{aligned}
x = 1/5 &= 0.2_{10} \\
&= 0.001100110011\ldots_2 \\
&\ominus 0.0011_2
\end{aligned}
$$

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Rounding

- Rounding should not introduce any systematic biases
- IEEE 754 defines 4 rounding modes:
  - to nearest (even in ties): default
  - to 0 (truncate)
  - to +Inf (round up)
  - to -Inf (round down)

Don’t test for equality!

- Because of this error in assignments, and other small perturbations we’ll see, testing for floating point equality is prone to failure.
- Generally don’t test for x== 0, or x==y
- abs(x) < tolerance, or abs(x-y) < tolerance

Rounding

- Can set rounding mode
  - C: #include <fenv.h>, fesetround()
    - FE_TONEAREST, FE_UPWARD, FE_DOWNWARD, FE_TOZERO
  - Fortran: use,intrinsic IEEE_ARITHMETIC
    - call IEEE_SET_ROUNDING_MODE(),
    - IEEE_DOWN, IEEE_UP, IEEE_TO_ZERO, IEEE_NEAREST

Machine Epsilon

- Let’s work in base 10, with mantisa precision=3 and exponent precision=2.
- (ignore denormal/ normalized for now; weird with non-binary)
- 1 + 0.001

Machine Epsilon

- Let's work in base 10, with mantisa precision=3 and exponent precision=2.
- (ignore denormal/normalized for now; weird with non-binary)
- 1 + 0.001
- There are numbers x such that 1 + x = 1 even though x isn't 0!

$$1 + 10^{-3}$$

$$\begin{array}{r} 1.00 \times 10^{0} \\ +\ 1.00 \times 10^{-3} \\ \hline \end{array}$$

$$\begin{array}{r} 1.00 \times 10^{0} \\ +\ 0.001 \times 10^{0} \\ \hline \ominus\ 1.00 \times 10^{0} \end{array}$$

Machine Epsilon

- Defined to be the smallest number s.t. 1+x != 1
- (or sometimes, the largest number s.t. 1+x = 1)
- single IEEE precision: ~1.19209e-07; double, ~2.22045e-16
- By repeated halving, try to see if you can calculate machine epsilon this way. What precision is default floating point number in python?

Machine Epsilon

```
In [4]: x = 1.

In [5]: while 1. + x > 1.:
   ...:     print x, 1.+x
   ...:     x = x / 2.
[...]
2.22044604925e-16 1.0
```

First lesson of floating point numbers

- Be wary of adding numbers that are potentially of very different magnitude
- Relative size ~ machine epsilon, regardless of absolute magnitude (eg, $10 + 10e_{mach} \sim 10$).
- What should we do when adding large series of numbers, even if of roughly same magnitude?

Subtraction: cancellation

- The same effect in opposite with subtraction

- Be wary subtracting very **similar** numbers.

$$
\begin{array}{rl}
 & 1.23 \times 10^{0} \\
- & 1.22 \times 10^{0} \\
\hline
\ominus & 1.00 \times 10^{-2}
\end{array}
$$

Subtraction: cancellation

- The same effect in opposite with subtraction
- Be wary subtracting very **similar** numbers.
- "catastrophic cancellation" - lose precision
- Dangerous in intermediate results

3 sig fig

3 sig fig

$$
\begin{array}{rl}
 & 1.23 \times 10^{0} \\
- & 1.22 \times 10^{0} \\
\hline
= & 1.00 \times 10^{-2}
\end{array}
$$

1 sig fig

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Things you **do** know

- Subtraction: if x, y floating-point representable numbers and x within a factor of 2 of y, then FP subtraction exact

$$x/2 < y < 2 \Rightarrow x \ominus y = x - y$$

- Rounding error when adding FP x and y is an FP number, and can be computed:

$$r = x + y - (x \oplus y) \Rightarrow r = b \ominus ((a \oplus b) \ominus a)$$

- subtraction is addition of a negative

- similar results exists for multiplication

Things you **do** know

- Math libraries typically provide functions (sin, cos, sqrt, pow, etc) results accurate to ~1-3 ulp, for given FP input
- For exact details, check manual

Be cautious, but don't despair

- FP errors are normally not a concern ~ 1 ulp
- Shouldn't normally be biased one way or another - error of N calculations ~sqrt(N) ulp
- (Note: iterate trillion computations in single precision - likely have O(1) errors)
- BUT need to be careful, especially of repeatedly iterated calculations or of awkward things early in a long calculation - if (eg) lose much precision early in a multi-stage computation

How do you know if there's a problem?

- Can test:
  - Change precision (single to or from double; fortran allows quad). Does answer significantly change?
  - Perturb calculation at ulp level by changing rounding behaviour. Does answer significantly change?
  - Perturb calculation by slightly changing inputs. Does answer significantly change?
- If you pass 3 tests, some evidence you're doing ok.

Floating Point and Compilers

- You generally want to turn on heavy levels of optimization when compiling (-O2, -O3); this can speed up your code significantly
- At -O3 levels (by convention), the compiler is allowed to re-order mathematical operations in such a way that, mathematically, give same answer
- But numerically may not!
- Overview of optimization flags for intel compilers: http://wiki.scinethpc.ca/wiki/images/7/77/Snug_techtalk_compiler.pdf

Floating Point and Compilers

- If your code is already demonstrated to be numerically stable, these perturbations shouldn't be a big issue.
- BUT:
  - Compiler may, by dumb luck, stumble on a reordering which is numerically unstable. Test with different optimization flags.
  - If your code includes something you've carefully written for numerical stability that you don't want reordered, put it in a separate file and compile it with -O2 or less

Floating Point and Compilers

- Other optimization flags include things like -ffast-math (or -funsafe-optimizations) which do more agressive changes
- -ffast-math likely does things like replace divisions with multiplication-by-reciprical, which is less accurate; may use less accurate but faster math functions. Worth trying, but be careful with this.
- -funsafe-math-optimizations: ditto.

Architecture and Floating Point

- In theory, all IEEE-754 compliant hardware should give same results.
- Mostly true; some small non-compliances here and there. Not normally a big worry (change in compilers more likely to cause numerical changes)
- Biggest difference: x86 does FP math on variables in registers in "extended precision" - 80 bits vs. 64.
- Higher precision, but depends on whether variables are in registers, etc.
- Can cause difference between x86 and other achitectures.
- Be aware of this.

Easiest way to avoid problem

- Don't write numerical code when you don't have to!
- If there exist numerical libraries for things you want to do (ODE, integration, FFTs, linear algebra, solvers), *use them*.
- Amongst other benefits, the numerical issues have been worked out in most mature, highly-used code bases.

Things to avoid

- Subtractions of like-sized variables early in calcuation
- Sumations of large amounts of numbers, or numbers of widely varying magnitudes
- Testing for exact floating-point equality

Things to do

- Try to keep values normalized in some sense so that all the values you're likely to deal with are of order unity (avoids machine epsilon problems)
- Try to use existing libraries when necessary
- Routinely test your code