AMath 483/583 — Lecture 6 — April 8, 2011

Today:

- Computer arithmetic
- Fortran subroutines and functions

Monday:

- Fortran array storage
- Fortran modules
- Multi-file Fortran codes

Read: Class notes and references.

Floating point real numbers

Base 10 scientific notation:

$$\texttt{0.2345e-18} = 0.2345 \times 10^{-18} = 0.0000000000000000002345$$

Mantissa: 0.2345, Exponent: -18

Binary floating point numbers:

Example: Mantissa: 0.101101, Exponent: -11011 means:

$$\begin{aligned} 0.101101 &= 1(2^{-1}) + 0(2^{-2}) + 1(2^{-3}) + 1(2^{-4}) + 0(2^{-5}) + 1(2^{-6}) \\ &= 0.703125 \;\; (\text{base } 10) \\ -11011 &= -1(2^4) + 1(2^3) + 0(2^2) + 1(2^1) + 1(2^0) = -27 \;\; (\text{base } 10) \end{aligned}$$

So the number is

$$0.703125 \times 2^{-27} \approx 5.2386894822120667 \times 10^{-9}$$

Floating point real numbers

Fortran:

real (kind=4): 4 bytes
This used to be standard single precision real

real (kind=8): 8 bytes
This used to be called double precision real

Python float datatype is 8 bytes.

8 bytes = 64 bits,

53 bits for mantissa and 11 bits for exponent (64 bits = 8 bytes).

We can store 52 binary bits of precision.

$2^{-52} \approx 2.2 \times 10^{-16} \implies$ roughly 15 digits of precision.

Floating point real numbers (8 bytes)

Since $2^{-52} \approx 2.2 \times 10^{-16}$
this corresponds to roughly 15 digits of precision.

We can hope to get at most 15 correct digits in computations.

For example:

```
>>> from numpy import pi
>>> pi
3.1415926535897931

>>> 1000 * pi
3141.5926535897929
```

Note: storage and arithmetic is done in base 2
Converted to base 10 only when printed!

Absolute and relative error

Let $\hat{z}=$ exact answer to some problem,
$z^*=$ computed answer using some algorithm.

Absolute error: $|z^*-\hat{z}|$

Relative error: $\dfrac{|z^*-\hat{z}|}{|\hat{z}|}$

If $|\hat{z}|\approx 1$ these are roughly the same.

But in general relative error is a better measure of how many correct digits in the answer:

Relative error $\approx 10^{-k} \quad \Longrightarrow \quad \approx k$ correct digits.

Absolute and relative error

Example:

Compute length of diagonal of 1 meter × 1 meter square.

True value: $\hat{z}=\sqrt{2}=1.4142135623730951\ldots$ meters
We compute $z^*=1.413$ meters

Absolute error: $|z^*-\hat{z}|\approx 0.0012135\approx 10^{-3}$ meters

Relative error: $\dfrac{|z^*-\hat{z}|}{|\hat{z}|}\approx\dfrac{0.0012135}{1.414}\approx 0.000858\approx 10^{-3}$

Note: Relative error is dimensionless.

The absolute and relative errors are both $\approx 10^{-3}$.

Roughly 3 correct digitis in solution.

Absolute and relative error

Exactly same problem but now measure in kilometers.

Compute length of diagonal of 0.001 km × 0.001 km square.

True value: $\hat{z}=\sqrt{2}\times 0.001=0.0014142135623730951\ldots$ km
We compute $z^*=0.001413$ km

Absolute error: $|z^*-\hat{z}|\approx 0.0000012135\approx 10^{-6}$ km

Relative error: $\dfrac{|z^*-\hat{z}|}{|\hat{z}|}\approx\dfrac{0.0012135}{1.414}\approx 0.000858\approx 10^{-3}$

The absolute error is much smaller than before
but there are still only 3 correct digits!

Absolute and relative error

Exactly same problem but now measure in nanometers.

Compute length of diagonal of 10^9 nm $\times 10^9$ nm square.

True value: $\hat{z}=\sqrt{2}\times 10^9=1414213562.3730951\ldots$ nm
We compute $z^*=1413000000$ nm

Absolute error: $|z^*-\hat{z}|\approx 1213562.373\approx 10^6$ nm

Relative error: $\dfrac{|z^*-\hat{z}|}{|\hat{z}|}\approx\dfrac{0.0012135}{1.414}\approx 0.000858\approx 10^{-3}$

The absolute error is much larger than before
but there are still 3 correct digits!

Machine epsilon (for 8 byte reals)

```
>>> y = 1. + 3.e-16
>>> y
1.0000000000000002

>>> y - 1.
2.2204460492503131e-16
```

Machine epsilon is the distance between 1.0 and the next largest number that can be represented: $2^{-52} \approx 2.2204 \times 10^{-16}$

```
>>> y = 1 + 1e-16
>>> y
1.0

>>> y == 1
True
```

Cancellation

We generally don't need 16 digits in our solutions

But often need that many digits to get reliable results.

```
>>> from numpy import pi
>>> pi
3.1415926535897931

>>> y = pi * 1.e-10
>>> y
3.1415926535897934e-10

>>> z = 1. + y
>>> z
1.0000000003141594    # lost several digits!

>>> z - 1.
3.141593651889707e-10  # only 6 or 7 digits right!
```

Rounding errors can cause big errors!

Example: Solve $Ax = b$ using Matlab, for

$$A = \begin{bmatrix} 1 & 2 \\ 2 & 4-10^{-12} \end{bmatrix}, \quad b = \begin{bmatrix} 5 \\ 10-2\times 10^{-12} \end{bmatrix}. \quad \text{Solution:} \quad \begin{bmatrix} 1 \\ 2 \end{bmatrix}.$$

```
>> format long e
>> A
A =
     1.000000000000000e+000     2.000000000000000e+000
     2.000000000000000e+000     3.999999999999000e+000

>> b
b =
     5.000000000000000e+000
     9.999999999998000e+000

>> x = A\b

x =
     9.982238010657194e-001    rel. error 0.00178
     2.000888099467140e+000    rel. error 0.00044
```

Note: This matrix is nearly singular (ill-conditioned).
Second column is almost a scalar multiple of the first.

Taylor series expansion for $\exp(x) = e^x$

The function $\exp(x)$ is provided by most computing languages.

But how is this computed??

Computer hardware can only do addition, subtraction, multiplication, division.

Other functions must be approximated by some algorithm using only these.

One useful tool is Taylor series expansions, e.g.

$$e^x = 1 + x + \frac{1}{2}x^2 + \frac{1}{3!}x^3 + \frac{1}{4!}x^4 + \cdots$$

Mathematically, this series converges for all x.

By taking enough terms, can make the error arbitrarily small.

But this is not true in finite precision computer arithmetic!

Cancellation

Example: Compute e^x using Taylor series when $x < 0$.

```
>>> import taylor;  from numpy import exp
>>> exp(-20.)
2.0611536224385579e-09

>>> taylor.exp(-20., 20)     # using N=20 terms
-21822593.77927747

>>> taylor.exp(-20., 100)    # using 100 terms
5.6218844721304176e-09

>>> taylor.exp(-20., 1000)   # using 1000 terms
5.6218844721304176e-09
```

Adding more terms does not help!!

Cancellation

Look more carefully at computation of $\exp(-7.)$:

```
True:        0.0009118819655545        0.0009118819655545

    j              j'th term                    partial_sum
    1        -7.0000000000000000        -6.0000000000000000
    2        24.5000000000000000        18.5000000000000000
    3       -57.1666666666666643       -38.6666666666666643
    4       100.0416666666666572        61.3749999999999929
    5      -140.0583333333333371       -78.6833333333333371
    6       163.4013888888888744        84.7180555555555372
    7      -163.4013888888888744       -78.6833333333333371
    8       142.9762152777777544        64.2928819444444173
    9      -111.2037229938271423       -46.9108410493827250
   10        77.8426060956790025        30.9317650462962774
```

6th term is $\frac{7^6}{7!} = \frac{7\cdot7\cdot7\cdot7\cdot7\cdot7}{6\cdot5\cdot4\cdot3\cdot2\cdot1}$, decrease only for $j > 7$.

Note: Partial sums about 10^5 times larger than answer,
So will lose at least 5 digits. Expect at most 10 digits correct.

Cancellation

Look more carefully at computation of $\exp(-7.)$:

```
True:        0.0009118819655545        0.0009118819655545

    j             j'th term                   partial_sum
    1       -7.0000000000000000       -6.0000000000000000
  ...
    6      163.4013888888888744       84.7180555555555372
  ...
   36        0.0000000000071284        0.0009118819666766
   37       -0.0000000000013486        0.0009118819653280
   38        0.0000000000002484        0.0009118819655764
   39       -0.0000000000000446        0.0009118819655318
   40        0.0000000000000078        0.0009118819655396
   41       -0.0000000000000013        0.0009118819655383
   42        0.0000000000000002        0.0009118819655385
   43       -0.0000000000000000        0.0009118819655385
   44        0.0000000000000000        0.0009118819655385
```

Note: Only 10 correct digits.
Adding more terms won't help!!

Cancellation

Better way to compute $\exp(-7.)$: $e^{-7} = 1/e^7$.

All terms in Taylor series for $\exp(7)$ are positive, no cancellation:

```
True:    1096.6331584284585006    1096.6331584284585006

    j              j'th term                    partial_sum
    1         7.0000000000000000         8.0000000000000000
    2        24.5000000000000000        32.5000000000000000
    3        57.1666666666666643        89.6666666666666572
    4       100.0416666666666572       189.7083333333333144
    5       140.0583333333333371       329.7666666666666515
    6       163.4013888888888744       493.1680555555554974
  ...
   41         0.0000000000000013      1096.6331584284575911
   42         0.0000000000000002      1096.6331584284575911
```

Note: 15 correct digits

```
>>> exp(-7.)
0.00091188196555451624

>>> 1. / taylor.exp(7.,40)
0.000911881965554517
```

Some disasters

Usually rounding errors are negligible compared to other errors introduced by numerical methods (e.g. truncating the Taylor series, discretizing a differential equation, etc.)

But some notable disasters have been caused by rounding error, see

http://www.ima.umn.edu/~arnold/disasters/

These issues are explored more in courses on numerical analysis.

Numerical analysis mostly deals with much more interesting things, but some understanding of the limitations of computer arithmetic is essential.

Fortran functions and subroutines

For now, assume we have a single file `filename.f90` that contains the main program and also any functions or subroutines needed.

Next week will see how to split into separate files.

Will also discuss use of modules.

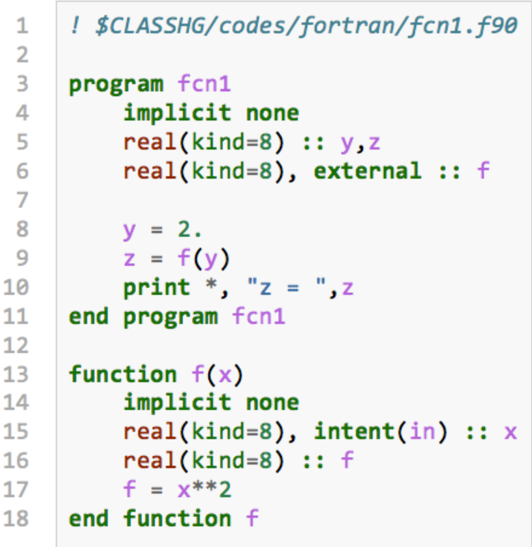
Functions take some input arguments and return a single value.

Usage: `y = f(x)` or `z = g(x,y)`

Should be declared as external with the type of value returned:

```
real(kind=8), external ::  f
```

Fortran functions



```fortran
! $CLASSHG/codes/fortran/fcn1.f90

program fcn1
    implicit none
    real(kind=8) :: y,z
    real(kind=8), external :: f

    y = 2.
    z = f(y)
    print *, "z = ",z
end program fcn1

function f(x)
    implicit none
    real(kind=8), intent(in) :: x
    real(kind=8) :: f
    f = x**2
end function f
```

Prints out:

```
z =      4.00000000000000
```

Fortran subroutines

Subroutines have arguments, each of which might be for input or output or both.

Usage: `call sub1(x,y,z,a,b)`

Can specify the intent of each argument, e.g.

```
real(kind=8), intent(in) :: x,y
real(kind=8), intent(out) :: z
real(kind=8), intent(inout) :: a,b
```

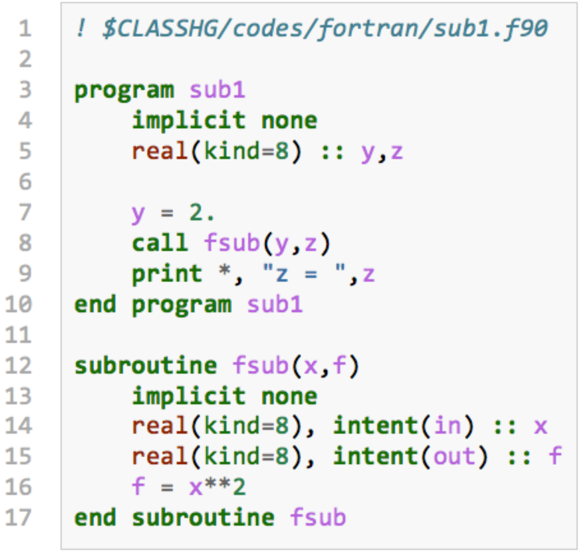
specifies that `x, y` are passed in and not modified,

`z` may not have a value coming in but will be set by `sub1`,

`a, b` are passed in and may be modified.

After this call, `z, a, b` may all have changed.

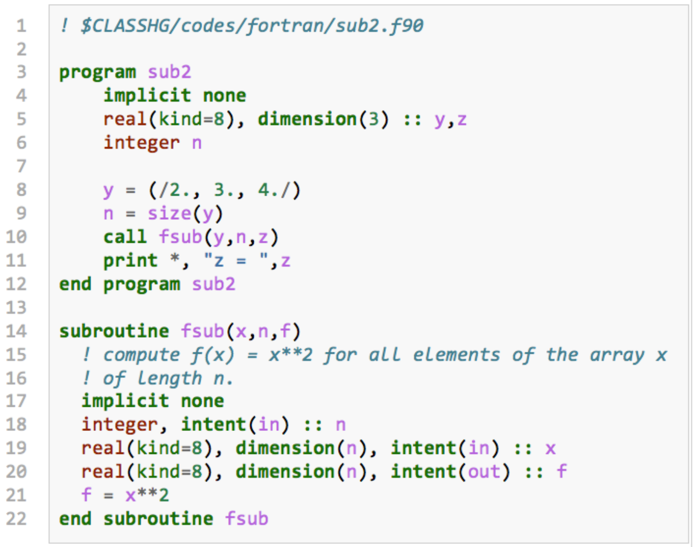
Fortran subroutines



```
! $CLASSHG/codes/fortran/sub1.f90

program sub1
    implicit none
    real(kind=8) :: y,z

    y = 2.
    call fsub(y,z)
    print *, "z = ",z
end program sub1

subroutine fsub(x,f)
    implicit none
    real(kind=8), intent(in) :: x
    real(kind=8), intent(out) :: f
    f = x**2
end subroutine fsub
```

Fortran subroutines

A version that takes an array as input and squares each value:



```
! $CLASSHG/codes/fortran/sub2.f90

program sub2
    implicit none
    real(kind=8), dimension(3) :: y,z
    integer n

    y = (/2., 3., 4./)
    n = size(y)
    call fsub(y,n,z)
    print *, "z = ",z
end program sub2

subroutine fsub(x,n,f)
  ! compute f(x) = x**2 for all elements of the array x
  ! of length n.
  implicit none
  integer, intent(in) :: n
  real(kind=8), dimension(n), intent(in) :: x
  real(kind=8), dimension(n), intent(out) :: f
  f = x**2
end subroutine fsub
```