Scientific Computing

Is an important part of of Computational Science that covers:

–Development of mathematical models (equations),

–Development of algorithms to solve equations numerically,

–Implementation of algorithms in software,

–Numerical simulation of physical phenomena using computer software,

–Interpretation, Validation and Visualisation of results.

History of SC

- Most of the concepts formulated 200 years ago by Newton, Gauss, Euler, Jacobi and many others.
- The motivation was obtaining approximate solutions for mathematical problems that arose in physics, astronomy and other fields of science.
- Efficient use of computational resources (pencil, paper, brain power),
- with the advent of computers the problem sizes are increasing,
- rounding errors are becoming critical, because the precision is not under human control,
- computation (simulation of reality) is becoming as important as measurements and theory.

Propagation Error

- Let ε express the relative error in representing a nonzero floating point number.
- The sum: $a(1 \pm \varepsilon) + b(1 \pm \varepsilon) = (a \pm a\varepsilon) + (b \pm b\varepsilon) =$
  $= (a + b) \pm \varepsilon\ (a + b) = (a+b)\ (1 \pm \varepsilon)$
  The sum error is in the same range as the error of factors. Similar is valid for difference, but suppose that a and b are of similar values then a-b $\approx$ 0 and e may become as large as result!
- The product: $a(1\pm \varepsilon)\ .\ b(1 \pm \varepsilon) = (a \pm a\varepsilon)\ .\ (b \pm b\varepsilon) =$
  $= ab \pm ab\varepsilon \pm ba\varepsilon \pm ab\varepsilon^2 \approx ab(1 \pm 2\varepsilon)$
  We get double error what leads to the pessimistic estimation of propagation error. Similar is valid for division.

Propagation Error (Cont.)

- For an exponent of n the relative error of result is n-times greater than initial error:
  $a(1 \pm \varepsilon)^n = a^n\ [(1 \pm n\varepsilon \pm n(n-1)\varepsilon\ ^2/2! \pm ...] \approx a^n\ (1 \pm n\varepsilon)$
- What happens if the exponent is smaller than 1? Is the error in result smaller?
- Similar is valid for m consecutive multiplication or division operations. Error can increase in the worst case for a factor of m.
- But in practical consecutive calculations we usually desire that the final result should have the similar absolute error as the less accurate input data.

Floating-Point Numbers

- Floating-point number system represents approximately the real number system.
- Floating point numbers are used in a similar way as scientific notation, with an exponent.
- Examples:
  $2347 = 2.347 * 10^3$,
  $0.0007396 = 7.396 * 10^{-4}$.
- The name floating-point is used because the decimal point floats as the power of 10 changes.

Floating-Point Numbers IEEE SP-normalized

- radix β=2,
- precision p=24 (23 bits for mantissa, 1bit for sign)
- exponent range [L=-126, U=127] (8 bits for exponent)
- 32 bits used for representation,
  $(1\ 00110001101001001001101\ 10010101)_2 =$
  $= -\ (2^{-3} + 2^{-4} + 2^{-8} + 2^{-9} + 2^{-11} + 2^{-14} + 2^{-17} + 2^{-20} + 2^{-21} + 2^{-23}) * 2^{-37} =$
  $(-\ 1.4113822957573241012596554355696 * 10^{-12})_{10}$
- the least significant bit in mantissa 1->0, the gap between two consecutive numbers:
  $2^{-23} * 2^{-37} = 2^{-60} =$
  $= 8.6736173798840354720596224069 * 10^{-19}$
- gaps are equally spaced between powers of β, but become smaller and smaller if we approaching to zero.

Floating-Point Numbers IEEE SP-normalized (Cont.)

- The number of all floating point numbers:
  $2 * (\beta-1) * \beta^{p-1} * (U-L+1) + 1 = 2^{24} * 254 + 1 = 4.261412865 * 10^{9}$
- Underflow (the smallest positive normalized number):
  $1.0 * \beta^{L} = 1.0 * 2^{-126} =$
  $= 1.17549435082228750796873653722 * 10^{-38}$
- Overflow level (the largest possible number):
  $\beta^{U+1} * (1- \beta^{-p}) = 1.1111... * 2^{127} =$
  $= 3.4028234663852885981170418348 * 10^{+38}$

Number of All FP Numbers

- sum of geometric series:
  $d_0 + d_0 * q + d_0 * q^2 + ... + d_0 * q^n$
  is: $Sn = d_0 * (1 - q^n) / (1 - q)$

- floating point representation of the largest number:
  $(d_o + d_1 \beta^{-1} + d_2 \beta^{-2} + ... + d_{p-1} \beta^{-(p-1)}) * \beta^U =$
  $= ((\beta-1) + (\beta-1)\beta^{-1} + (\beta-1)\beta^{-2} + ... + + (\beta-1)\beta^{-(p-1)}) * \beta^U$
  we have: $n=p$, $d_0 = (\beta-1)$, and $q = \beta^{-1}$ so the sum is:

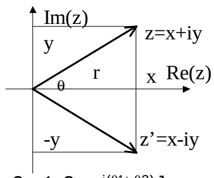
  $((\beta-1) * (1 - \beta^{-p}) / (1 - \beta^{-1})) * \beta^U =$
  $= ((\beta-1) * \beta * (\beta^p - 1) / (\beta-1) * \beta^p) * \beta^U =$
  $= \beta^{-(p+1)} * (\beta^p - 1) * \beta^U =$ $\beta^{U+1} (1- \beta^{-p})$

Machine Precision

- Determines the maximum possible relative error in representing a nonzero real number.
- We know that the smallest positive normalized number is:
  $1.0 * \beta^L = 1.0 * 2^{-126} =$
  $= 1.17549435082228750796873653722 * 10^{-38}$
- The nearest neighbouring number:
  $1.00000000000000000000001 * \beta^L = (1.0+2^{-23}) * 2^{-126} =$
  $= 1.17549449095213394045044362950 * 10^{-38}$
- The difference and relative error (constant for all FP numbers):
  $diff=1.401 * 10^{-45}$, $rel\_err=1.192 * 10^{-7}$
  what means that we have about 7 digits of precision in SP.
- Machine precision with rounding to nearest in IEEE SP:
  $\varepsilon_{mach} = 1 * \beta^{1-p} = 1 * 2^{-23} = 5.9604644775390625 * 10^{-8}$

Complex Numbers

- A given complex number z can be expressed as $z=x + i*y$, where $x=Re(z)$ and $y=Im(z)$ are real numbers and $i=sqrt(-1)$.
- x and y are real and imaginary parts, respectively, of z. A complex number can be real if $Im(z)=0$ or purely imaginary if $Re(z)=0$.
- Complex conjugate $z' = x - iy$
  $z*z' = x^2+y^2$ $r=|z|=sqrt(x^2+y^2)$
- Complex arithmetic more costly than real arithmetic.
  $z1*z2=(x1x2-y1y2)+i(x1y2+x2y1)$]
- Polar presentation:
  $z=r*(\cos\theta + i*\sin\theta) = re^{i\theta}$ [now: $z1*z2=r1r2\, re^{i(\theta1+\theta2)}$]



Practical Advises on Software

- FORTRAN (reliable, tuned, efficient BUT expensive, restrictive, not available for all machines),
- C, C++ (free, versatile , popular, available on all platforms) ,
- TRANSLATORS (f2c) opposite array storage convention, function calls,
- MATLAB (high-level, interactive, built-in graphic, easy to learn)