Class 5. Data Representation and Introduction to Visualization

Visualization

- Visualization is useful for:
  1. Data entry (initial conditions).
  2. Code debugging and performance analysis.
  3. Interpretation and display of results.
- Our focus will be #3. The computational astrophysicist can either:
  1. Develop new visualization software tailored to problem under study.
  2. Use an existing software package.

Plotting 1-D data

- Function of one variable only: $f(x)$ *vs.* x.
- Examples: `sm`, `gnuplot`, `xgobi`, IDL, etc.
- Minimum requirements:
  - Read data from file.
  - Perform arithmetic manipulation of data.
  - Multiple data sets on plot.
  - Multiple plots on page.
  - Add text to plots.

Plotting 2-D data

- Function of 2 variables, i.e. $f(x, y)$.
- If f is a scalar quantity, can:
  1. Make image.
     - Represent each (x, y) data point by one or more pixels on screen.
     - Use integer value to represent data value at (x, y) point (8 bit: 0–255; 24-bit: 0–16.8 million).
  2. Make contour plot.
     - Contours are isosurfaces of data.
  3. Make 3-D surface plot.
     - Use (x, y) as 2 coordinates, f as third coordinate, plot surface.

- If f is a vector quantity, i.e. $\mathbf{f}(x, y)$, can:
  1. Plot vectors directly (as arrows).
     – Can be hard to see.
  2. Plot streamlines.
     – Contours of Φ, where $\mathbf{f} = \boldsymbol{\nabla}\Phi$.
- 2-D plotting packages include `sm`, `gnuplot`, `xgobi`, IDL, `ximage`, NCAR graphics, etc.

Plotting 3-D data

- Function of 3 variables, i.e. $f(x, y, z)$.
- If f is a scalar quantity, can:
  1. Plot 2-D slices.
     – E.g. faces of cube.
  2. Plot isosurfaces.
     – These are now 3-D surfaces. Can use wireframe of polygons. Can shade with second variable $g(x, y, z)$.
  3. Plot volumetric rendering.
     – Solve transfer equation ("ray tracing") using emissivity proportional to data value.
- Standard algorithms exist for 3-D rendering, including shadowing, hidden surface removal, etc. Often implemented in hardware. Also have "dynamic/interactive" visualization: rotation, etc.
- If f is a vector quantity, i.e. $\mathbf{f}(x, y, z)$, can:
  1. Plot 3-D vectors on 2-D slice.
  2. Plot streamlines in 3-D.
- 3-D plotting packages include `tipsy`, `xgobi`, IDL, NCAR graphics, `xdataslice`, etc.

Animation

- If any one of the coordinates of data in a plot is time, it makes sense to render images as a time sequence, e.g. make animation.
- The eye is very sensitive to motion, can discover much detail using animations.
- Animation formats include `MPEG`, `FLI`, `QT`, `AVI`, `GIF`, plus many custom formats.
- Animation players include `mpeg_play`, `xanim`, `quicktime`, `gifview`, etc.
  – Often built into web browsers.

Data Representation

- Computers store data as different variable types, e.g. integer, floating point, complex, etc.
- Different machines have different wordlengths, e.g. 4-byte `ints` on a 32-bit machine (Pentium), 8-byte `ints` on a 64-bit machine (G5).
- This makes (binary) data non-portable.

Integers

- All data types represented by 0's and 1's.
- An integer value:

$$j = \sum_{i=1}^{N} s_i \times 2^{N-i}$$

  - $N = \#$ of bits in word.
  - s_i = value of bit i in binary string s.
- E.g., $0\ 0\ 0\ 0\ 0\ 1\ 1\ 0 = 2^2 + 2^1 = 6$ for 8-bit word.
- Use "two's complement" method for sign (see below).
- Largest value that can be represented is $2^N - 1$.
- For 32-bit word this is 4,294,967,295.
- Arithmetic with integers is exact, except:
  - when division results in remainder, or
  - result exceeds largest representable integer.

    E.g. $2 \times 10^9 + 3 \times 10^9 =$ overflow error.
- Note multiplication (division) by 2's can be achieved by left-shift (right-shift), which is very fast (in C, use the $<<$ ($>>$) operator).

Two's complement

- Exploits finite size of data representations (cyclic groups) and properties of binary arithmetic.
- To get negative of binary integer, invert all bits and add 1 to the result.

	invert bits:	1 1 1 1 1 1 1 0
E.g., $1 = 0\ 0\ 0\ 0\ 0\ 0\ 0\ 1$ in 8-bit.	add 1:	$\underline{0\ 0\ 0\ 0\ 0\ 0\ 0\ 1}$
	result:	$1\ 1\ 1\ 1\ 1\ 1\ 1\ 1 = -1$

- In 8 bits, signed `char` ranges from -128 to $+127$.

Negative powers of 2

- Binary notation can be extended to cover negative powers of 2, e.g. "110.101" is:

  $1 \times 2^2 + 1 \times 2^1 + 1 \times 2^{-1} + 1 \times 2^{-3} = 6.625.$

- Can represent real numbers by specifying some location in the word as the "binary point" ("fixed-point representation").

- In practice, use some bits for an exponent ("floating-point representation").

Floats

- For most machines these days, real numbers are represented by floating-point format:

$$x = s \times M \times B^{e-E}$$

$$\begin{aligned} s &= \text{sign} & B &= \text{base (usually 2, sometimes 16)} \\ M &= \text{mantissa} & e &= \text{exponent} \\ E &= \text{bias, usually 127.} \end{aligned}$$

- In past, manufacturers used different number of bits for each of M and e, resulting in non-portable code.

- Currently, most manufacturers adopt IEEE standard:

  - s = first bit.
  - Next 8 bits are e. ($e = 255$ reserved for inf & NaN.)
  - Last 23 bits are M, expressed as a binary fraction, either 1.F, or, if $e = 0$, 0.F (in which case $E = 126$), where F is in base 2.

  E.g., 0 10000001 10100000000000000000000 $= (+1)\left[2^{(129-127)}\right](1+0.5+0.125) = 6.5$.

- Largest single-precision float $f_{\max} = 2^{127} \times (1+1/2+1/4+\cdots+1/2^{23}) \approx 3.4028235 \times 10^{38}$ (just under 2^{128}).

- Smallest (and least precise!) $f_{\min} = 2^{-149} \approx 10^{-45}$.

Round-off error

- Not all values along real axis can be represented.

- There are 10^{38} integers between $f_{\min}$ and $f_{\max}$, but only $2^{32} \approx 10^9$ bit patterns.

- Values $< |10^{-45}|$ result in "underflow" error.
- If value cannot be represented, next nearest value is produced. Difference between desired and actual value is called "round-off error" (RE).
- Smallest value e_m for which $1 + e_m > 1$ is called "machine accuracy," typically $2^{-23} \sim 10^{-7}$ for 32 bits.
- Double precision greatly reduces e_m ($\sim 10^{-16}$). (In this case the 64 bits are divided into 1 sign bit, 11 exponent bits, and 52 mantissa bits; the bias is 1023.)
- RE accumulates in a calculation:
  - Random walk: total error $\sqrt{N} e_m$ after N operations.
  - But algorithms rarely random, giving linear error $N e_m$.
- Subtraction of two very nearly equal numbers can give rise to large RE.

  E.g., solution of quadratic equation...

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

  ...can go badly wrong whenever $ac \ll b^2$ (Cf. PS#2).

- RE cannot be avoided—it is a consequence of using a finite number of bits to represent real values.

Truncation error

- In practice, most numerical algorithms approximate desired solution with a finite number of artithmetic operations, e.g.,
  - evaluating integral by quadrature;
  - summing series using finite number of terms.
- Difference between true solution and numerical approximation to solution is called "truncation error" (TE).
- TE exists even on "perfect" machine with no RE.
- TE is under programmer's control; much effort goes into reducing it.
- Usually RE and TE do not interact.
- Sometimes TE can amplify RE until it swamps calculation. The solution is then called <u>unstable</u>.

  E.g., integer powers of Golden Mean (Cf. PS#2).