Dealing with quantitative data and problem solving…life is a story problem!

A large portion of science involves quantitative data that has both value and units.

- Units can save your butt!
- Need handle on metric prefixes

Dimensional Analysis

- Devise calculation using conversion factors so unneeded units cancel and necessary units are left behind.
- How many cm are in 1 km?

- Appendix A-5
- Practice, Practice, Practice!!!

TABLE 1.2 SI Prefixes

Multiple	Prefix
10^{18}	exa (E)
10^{15}	peta (P)
10^{12}	tera (T)
10^{9}	giga (G)
10^{6}	mega (M)
10^{3}	kilo (k)
10^{2}	hecto (h)
10^{1}	deca (da)
10^{-1}	deci (d)
10^{-2}	centi (c)
10^{-3}	milli (m)
10^{-6}	micro (μ)[a]
10^{-9}	nano (n)
10^{-12}	pico (p)
10^{-15}	femto (f)
10^{-18}	atto (a)

[a] The Greek letter μ (pronounced "mew").

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Attacking Quantitative Problems

1. Read the question
2. Identify the required quantity (and units)
3. Devise a way to use given information to get required quantity (and units)
   - set up necessary calculations
   - Check to be sure you get the correct units!
4. Insert values into equations and solve
5. Look at the answer
   - is it reasonable (order of magnitude, unit)?
6. Read the question again

Example:

- If the diameter of a single carbon atom is 154 pm, how many atoms would be in a line 100.0 μm long (about the diameter of a human hair)?
- How much would this line weigh if a single carbon atom weighs 1.993×10^{-23}g?

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What can a result tell us?

What is the "truth"?

- We don't (and can't) determine the "true value" of any component in a mixture.
  - All measurements have some associated error (uncertainty).
  - Representation of results must illustrate this error; otherwise value is useless!

- We can work to understand (and improve) the precision of a measurement.
  - Precision =

- Comparing multiple methods increases confidence in the accuracy of our results.
  - Accuracy =

Representation of Quantitative Data

Significant Figures: Number of digits necessary to present a result with the appropriate accuracy.

- *Last digit has uncertainty, at least ±1!*

- Results are presented to the appropriate number of significant figures, and often accompanied by the error in the final digit.

  Value ± Error
  e.g. 102.5 ± 0.1 ppm

- When rounding, look at all digits beyond the last place needed.

- Always round values that are exactly halfway to the nearest ***even*** digit.

  12.250 → 12.2
  12.350 → 12.4
  12.250001 → 12.3

Guidelines for Sig. Figs.

When looking at a number:

1. all nonzero digits are significant,
2. all zeros that appear between nonzero digits of a number are significant,
3. all zeros at the end of a number on the right hand side of the decimal point are significant,
4. all other zeros are not significant.

Examples: How many significant figures in each value?

14600
0.0146
14060.0
10460

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Sig. Figs. and Calculations

In doing calculations, the number sig figs is limited by the least certain piece of data.

- <u>Addition/Subtraction</u>
- <u>Multiplication/Division</u>

- Example: How many sig. figs. should be in the answers to the following:

  126.23 + 0.0147 =
  58.6 x 3.1 =

- **NOTE:** Wait to truncate results until the end of the calculation! WHY???

- Indicate "extra" digits by subscripting:
- Exact numbers don't impact sig. figs.

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Types of Error (Uncertainty)

- **Uncertainties fall into two main classes:**
  - Systematic Error:
  - Random Error
- **Two general approaches to quantifying error:**
  - Absolute Uncertainty
  - Relative Uncertainty, (% Relative Uncertainty)

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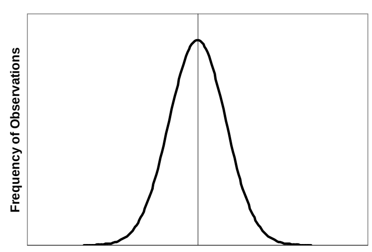
Statistics and Quantitative Data

- Statistics allow an estimation of uncertainty in our data.
  - **AS LONG AS:**
- Foundation of statistics: Normal Distribution
- Two parameters define the distribution:
  - μ:
  - σ:
- Statistical analyses relate experimental data to this "ideal" distribution.
  - BUT, there are some challenges!



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Statistics in Practice: Remember the key assumption!

Describing the precision of our data.

- *Average, or Arithmetic Mean:*
  - *n* is the number of samples

$$\bar{x} = \frac{\sum_i x_i}{n}$$

- *Sample Standard Deviation:*

$$s = \sqrt{\frac{\sum_i (x_i - \bar{x})^2}{n - 1}}$$

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Describing the "uncertainty" in our data. How good is it?

- When we determine an average (with some associated error), how sure are we that the "true value" is close to this average?
  - What factors influence this confidence?

- The most common statistical tool for determining that the "true" value is close to our calculated mean is the **confidence interval.**
  - The *confidence interval* presents a range about the mean, within which there is a fixed probability of finding the "true value", m.

$$\mu = \bar{x} \pm \frac{ts}{\sqrt{n}}$$

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More on Confidence Limits

- Values for t are tabulated based on several confidence levels and various numbers of degrees of freedom.

	Confidence Level (%)						
Degrees of Freedom	**50**	**90**	***95***	**98**	**99**	**99.5**	**99.9**
3	0.765	2.353	*3.182*	4.541	5.841	7.453	12.924
120	0.677	1.658	*1.980*	2.358	2.617	2.860	3.373

  – **NOTE:** even though the number of measurements (n) is used in the CI calculation, t is determined based on the *degrees of freedom* (n-1).

- Let's look at some data:

  What is the average?
  What is the standard deviation (s)?
  What is the 95% confidence limit?

4.9761	4.9693	4.9713	4.8903	4.9631
4.9551	4.9586	5.0012	4.9781	4.9895

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Error Propagation
(*aka propagation of uncertainty*)

How do errors in individual values affect an analysis?

– Effects depend on how the data is used.
– "Rules" come from calculus!

Error Propagation in Addition and Subtraction:

– Overall error is based on the absolute uncertainties of individual values.

$$e_4 = \sqrt{e_1^{\,2} + e_2^{\,2} + e_3^{\,2}}$$

– Example:

$$\begin{array}{r} 12.4 \pm 0.2 \\ 5.7 \pm 0.1 \\ +\quad 1.43 \pm 0.04 \\ \hline 19.53 \pm ??? \end{array}$$

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More Error Propagation

Error Propagation in Multiplication and Division

– Concept is the same as addition and subtraction, except *relative uncertainties* are used

$$\frac{e_4}{v_4} = \sqrt{\left(\frac{e_1}{v_1}\right)^2 + \left(\frac{e_2}{v_2}\right)^2 + \left(\frac{e_3}{v_3}\right)^2}$$

$$\%e_4 = \sqrt{(\%e_1)^2 + (\%e_2)^2 + (\%e_3)^2}$$

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