12.010 Computational Methods of Scientific Programming

Lecturers
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Mathematica

- Look in more detail at some of the programming features in Mathematica
- There are many of these features and in all Mathematica expressions there are Function names and “short-hand” symbols
- The + usage is actually a function Plus, * is Times
- Use of FullForm shows full form of expressions
Flow control

- If statement form:
  - `If[condition, t, f]` gives `t` if condition evaluates to True, and `f` if it evaluates to False.
  - `If[condition, t, f, u]` gives `u` if condition evaluates to neither True nor False.
- The standard conditions tests are `==`, `!=`, `<`, `<=`, `>`, `>=`
- Multiple test are `&&` (and) `||` (or)
- It also possible combine:
  - `if[ 7 > 6 > 5, ..]` rather than `if[ 7 > 6 && 6 > 5, ..]`
- Which allows a range of actions:
  - `Which[{test1, value1, test2, value2, test2, value2}]`
- Switch allows action based on result of expression:
  - `Switch[expr, form1, value1, form2, value2]`
- Examples in `12.010.Lec13.nb`

Loop structures

- Do structure: Most general structure
  - `Do[expr, {i, imin, imax, di}, {j, jmin, jmax, dj}, ... ]`
  - This would loop through values of `j` from `jmin` to `jmax` in increments of `dj`, for each value of `i` which would loop from `imin` to `imax` in increment of `di`.
- If the increment is not given 1 is assumed, if `imax` is not given, then loops from 1 to `imin`. If only 1 argument is given, `expr` is evaluated that many times.
- While[ test, body] executes code in body (statements are separated by :) while ever test is true.
  - `Return[val]` can be used to return a value from the `body` code;
  - `Break[]`can be used to exit body
- For[start, test, incr, body] executes start, then repeatedly evaluates body and incr until test fails to give True
- Mathematica does have a `Goto[tag]` statement using `Label[tag]`
Functions

- Function[body] or body& is a pure function. The formal parameters are # (or #1), #2, etc.
- Function[x, body] is a pure function with a single formal parameter x.
- Function[{x1,x2,…}, body] is a pure function with a list of formal parameters.
- If the body is more than one statement, normally there would be a Return[..] call to set the quantity returned form the call.
- Map[f, expr] or f /@ expr applies f to each element on the first level in expr.
- Apply[f, expr] or f @@ expr replaces the head of expr by f. This is basically a way of changing what something is in Mathematica e.g., if expr is a list {…}, it can be changed to Times (multipl...)

Pattern Matching

- _ or Blank[] is a pattern object that can stand for any Mathematica expression.
- _h or Blank[h] can stand for any expression with head h. We used this in lecture 6 to x_Integer for an integer argument.
- __h or BlankSequence[h] can stand for any sequence of one or more expressions, all of which have head h.
- g[x_, y___] := x + y; g[a, b, c] yield a+b+c
- Replace and Rules: -> (arrow on Palette) applies a rule for to convert lhs to rhs, /. is the replace all e.g. 1 + x /. x -> a yields 1+a (same as ReplaceAll[1 + x, x -> a])
- There are many more forms of rules and replacements that are given in the Pattern Matching and Rule applications in the Programming section of the Mathematica help.
Format types

• Mathematica offers many different types of ways to display results and convert to different formats
• These are given in the Format Types under Input Output sections of the Built in Functions
• Some examples are TableForm, MatrixForm, TreeForm
• \texttt{N[expr]} gives the numerical value of expr.
• \texttt{N[expr, n]} attempts to give a result with n-digit precision.

Files and directories

• \texttt{Directory[ ]} - give your current working directory
• \texttt{SetDirectory["dir"]} - set your current working directory
• \texttt{FileNames[ ]} - list the files in your current working directory
• \texttt{FileNames["form"]} - list the files whose names match a certain form
• \texttt{<<name} - read in a file with the specified name (Get)
• \texttt{<<context`} - read in a file corresponding to the specified context
• \texttt{CopyFile["file1","file2"]} - copies file1 to file2
• \texttt{DeleteFile["file1"]} - deletes the file.
• \texttt{Input["prompt"]} is used to read information from the keyboard
Final Comments

• Users of Mathematica need to understand the basics of the syntax of the program. The online help however provides the details of the capabilities of the program.
• Built-in Functions is grouped by
  Numerical Computation
  Algebraic Computation
  Mathematical Functions
  Lists and Matrices
  Graphics and Sounds
• Program development should be knowing what you want to do and then finding the Functions that, in combination, will do the task.
• With Notebooks, you can keep track and comment on the way the program works.
• Homework #4 will be due Thursday Nov 10.