12.010 Computational Methods of Scientific Programming
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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:
  \[\text{If[condition, t, f]}\] gives \(t\) if condition evaluates to True, and \(f\) if it evaluates to False.
  \[\text{If[condition, t, f, u]}\] 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\(\ [\ 7 > 6 \&\& 6 > 5, \ldots]\)
• Which allows a range of actions:
  Which[\text{test1, value1, test2, value2, test2, value2}]
• Switch allows action based on result of expression:
  Switch[\text{expr, form1, value1, form2, value2}]
• Examples in 12.010.Lec13.nb
Loop structures

• Do structure: Most general structure
  
  \[
  \text{Do[}\ expr, \{i, \text{imin}, \text{imax,di}\}, \{j, \text{jmin}, \text{jmax,dj}\}, \ldots \]\n  
  This would loop through values of \( j \) from \( \text{jmin} \) to \( \text{jmax} \) in increments of \( \text{dj} \), for each value of \( i \) which would loop from \( \text{imin} \) to \( \text{imax} \) in increment of \( \text{di} \).

• If the increment is not given 1 is assumed, if \( \text{imax} \) is not given, then loops from 1 to \( \text{imin} \). If only 1 argument is given, \( \text{expr} \) is evaluated that many times.

• While[ test, \( \text{body} \)] executes code in body (statements are separated by ;) while ever test is true. Return[\text{val}] can be used to return a value from the \( \text{body} \) code; Break[] can be used to exit body

• For[start, test, incr, \( \text{body} \)] 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. Body can have multiple statements separated by ;
• 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 (multiply)
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`.
- `N[expr]` gives the numerical value of `expr`.
- `N[expr, n]` attempts to give a result with n-digit precision.
Files and directories

- Directory[ ] - give your current working directory
- SetDirectory["dir"] - set your current working directory
- FileNames[ ] - list the files in your current working directory
- FileNames["form"] - list the files whose names match a certain form
- <<name - read in a file with the specified name (Get)
- <<context` - read in a file corresponding to the specified context
- CopyFile[“file1”,"file2"] - copies file1 to file2
- DeleteFile[“file1”] - deletes the file.
- 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 8, 2007.