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
  \[ \text{Do}[\text{expr}, \{i, \text{imin}, \text{imax}, \text{di}\}, \{j, \text{jmin}, \text{jmax}, \text{dj}\}, \ldots] \]
  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[\text{tag}] statement using Label[\text{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.
- \( \text{N[expr]} \) gives the numerical value of \( \text{expr} \).
- \( \text{N[expr, n]} \) 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
Graphics

- Mathematica supports a variety of graphics plots through its basic plot command.
- Simple plots can be modified with options given in the plot command.
- Mathematica 6.0 has a new Manipulate command
  Syntax of command: The variable a here is the one that can be manipulated between values of 0 and 2.
  Manipulate[Plot[Sin[x (1 + a x)], {x, 0, 6}], {a, 0, 2}]
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 13, 2008.