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12.010 Computational Methods of Scientific Programming
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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`. 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 from 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

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.
- Mathematic 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.