Vojtěch Janoušek & Ondrej Lexa:

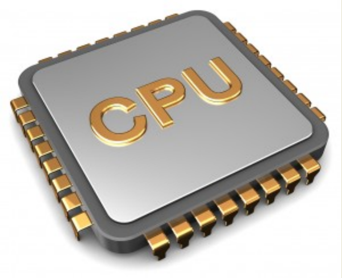
What is a computer program? Principles of algorithmization

Programming languages

Programming language

Is a system for describing computation in machine-readable and, at the same time, human-readable form

- High-level languages
  - the balance is in favor of the human comfort (e.g., *Basic, Pascal, Fortran…*)
- Low-level languages
  - assembly languages and other languages (e.g., *C++*) designed to more closely resemble the computer's processor (CPU) instruction set
  - powerful, quick (used, e.g., in programming operation systems, applications)



- Interpreted
  - each command is executed directly by the interpreter
  - slow; advantages = produce smaller, portable code
- Compiled
  - program has to be previously compiled into the machine language
  - bigger, specific to the given system (CPU); advantage = speed

Programming languages

Scientific programming languages

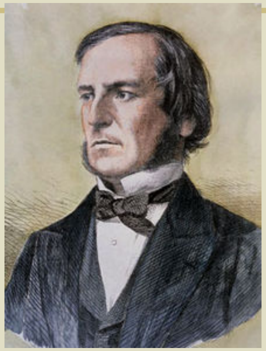
- designed esp. for mathematical computations
- extensive use of matrices
- sophisticated graphical functions
- high-level graphical output
- (statistical tools)
- interpreted, direct vs. batch use (scripting)
- e.g. *ALGOL, FORTRAN, Python, R, Matlab, Julia*

Programming language paradigms

- **Imperative / procedural**
  - command-driven or statement-oriented languages *(e.g., Fortran, C, Pascal)*
  - a program consists of a sequence of statements, the execution of each changes the machine state
- **Functional**
  - everything is viewed as a large function *(e.g., Scheme, LISP)*
- **Declarative** (rule-based)
  - a program consists of a set of rules and it continuously checks whether a particular condition is true
  - if so, the appropriate actions are performed (e.g., *Prolog*)
- **Object-oriented**
  - data structures and algorithms support the abstraction of data
  - the aim is to allow the programmer to use data in a fashion that closely represents their real world use

Many of the widely used programming languages are multi-paradigm, i.e. support object-oriented programming (OOP) to a greater or lesser degree, typically in combination with imperative, procedural programming.

Fundamental data types



George Boole (1815–1864)

Variables

Symbolic name, referring to a storage (memory) which contains some known or unknown quantity of information (a *value*)

Variable types

- **Numeric** (integer, float, real…)
- **Character / text / string**
- **Logical / Boolean**
  only two values are allowed, logical TRUE or FALSE

Many (esp. older) programming languages require first a strict declaration of the variable type (e.g., Pascal)

Modern ones allow an easy conversion, though:
e.g. in R *as.numeric, as.character*
and this is often done automatically
by the interpreter

John von Neumann (1903–1957)

Fundamental data types

Bit = a basic unit of digital information, 0 or 1

Byte = commonly consists of 8 bits

In use are prefixes kilo (10^3 = kB vs. 2^{10}= 1024 = kiB), mega, giga, tera etc.

Decimal positional numeral system (0–10)

Decimal number	**1**	**5**	**1**	**1**	**9**
Multiply by	**10^4**	**10^3**	**10^2**	**10^1**	**10^0**
Decimal result	**10000**	**5000**	**100**	**10**	**9**

Decimal representation of the number 15 119

Binary positional numeral system (0–1)

Binary number	0	0	0	**1**	0	**1**	**1**	0
Multiply by	2^7	2^6	2^5	2^4	2^3	2^2	2^1	2^0
Decimal result	0	0	0	**16**	0	**4**	**2**	0

Binary representation of the decimal number 22 is 00010110
Eight bits can express decimal numbers of 0–255

Fundamental data types

Hexadecimal positional numeral system (0–F; A = 10, B = 11...)

Hexadecimal number	**3**	**B**	0	**F**
Multiply by	**16^3**	**16^2**	16^1	**16^0**
Decimal result	**12288**	**2816**	0	**15**

Hexadecimal representation of the number 15119 is #3B0F, &3B0F etc.

Conversion from hexadecimal to binary system

Hex	3				B				0				F			
Bin	0	0	1	1	1	0	1	1	0	0	0	0	1	1	1	1

Just interpret each of the hexadecimal “digits” as four binary ones

Binary representation of the number 15119 (#3B0F) is thus 0011 1011 0000 1111

Fundamental data structures

Types of data structures I.

- o **Homogenous**
  contain elements of the same type
- o **Heterogeneous**
  may contain a mixture of elements of various types

https://en.wikipedia.org/wiki/Data_structure

Types of data structures II.

- **1D (linear)**
  - o **single value (scalar)**
  - o **vector**
    sequence of ordered elements, often of the same type
    these elements can be accessed using an integer index, or by name, specifying which element is required
  - o **categorical**
    can attain only a discrete number of values from a certain dictionary/ look up table (e.g. names of countries)

    in R they are called *factors* and all possible discrete values are *levels*

Fundamental data structures

- **1D (linear) [CONTD.]**
  - **list**
    linear collection of data elements of any type, whereby each has itself a value (can be even other list – lists are recursive structures)
  - **record**
    aggregate data structure, typical in database use
    each record is a value that contains other values, typically in fixed sequence and often indexed by names
- **2D**
  - **matrix / array**
    ordered elements are accessed using an integer index, or by name, to specify which element is required
- **Multi-dimensional**
  - **(multidimensional) array**

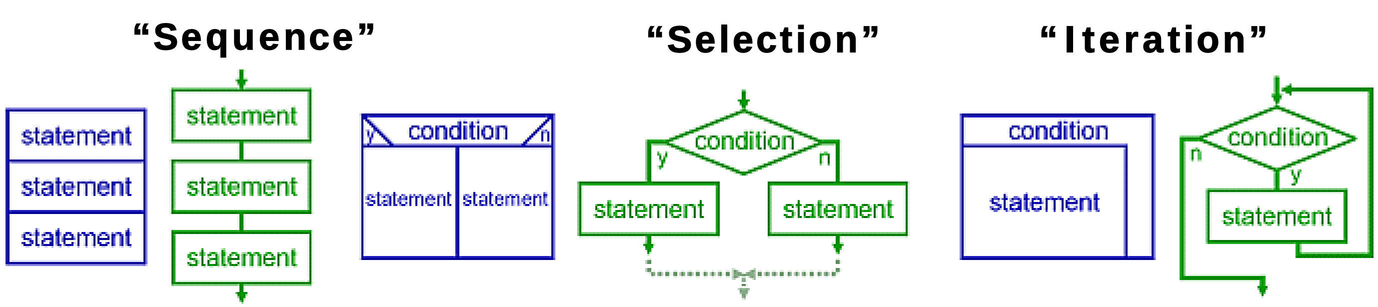
Modern languages allow an easy conversion: e.g. in R *as.matrix, as.vector,…*

This conversion can be even done automatically by the interpreter
(e.g., a matrix with a single row or column becomes a vector in R)

Building blocks of a computer program

Typical computing language contains commands for:

- **Data input**
  from the keyboard, a file, (Internet) connection, or some other device
- **Output**
  on the screen, into a file or to some other device
- **Procedures** that modify data (incl. basic arithmetical operations) **(“Sequence”)**
- **Conditional execution (“Selection”)**
  appropriate sequence of statements is executed only if some condition is fulfilled
- **Loop (“Iteration”)**
  performs some action repeatedly, e.g., given number of times or till something happens (e.g.. variable changes or some event occurs)



Nassi–Shneiderman diagrams (blue) and **flow charts** (green)

Flowcharts

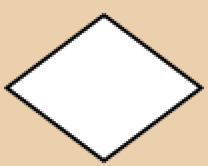
Flowcharts

- Once dominated basic computer science textbooks
- Are used in designing and documenting any complex process
- Consist of various boxes connected by arrows, showing the flow of the process being coded (= flow lines)

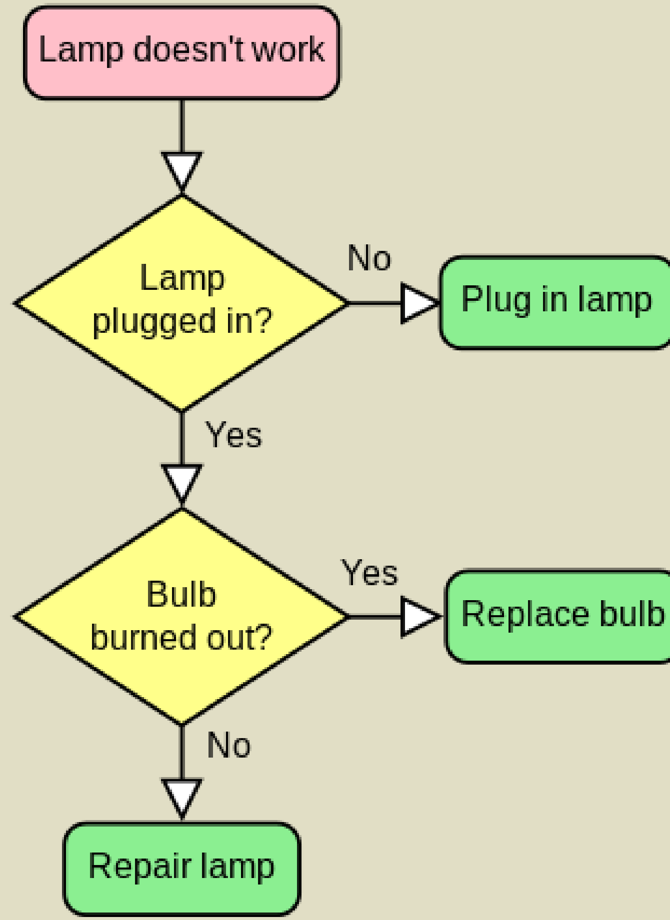
The most common types of boxes are:

– start and end symbols (circle, oval or rounded rectangle)

– processing step, usually called activity (rectangular box)



– conditional or decision (diamond = rhombus) where a decision is necessary, commonly a *Yes/No question* or *TRUE/FALSE test*



https://en.wikipedia.org/wiki/Flowchart

Flowcharts

– Subroutine (procedure)

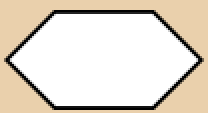
(rectangle with double-struck vertical edges)

- pre-defined complex processing steps
- may be detailed in a separate flowchart

– Input/Output

(parallelogram)

- receiving data or displaying processed data

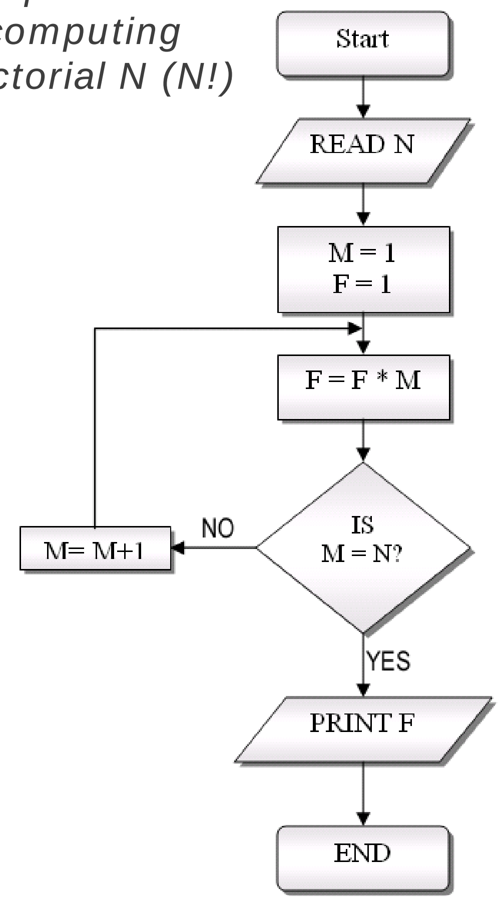


– Prepare conditional

(hexagon)

- operations only initializing a value for a subsequent conditional step or decision
- e.g., in conditional looping

A simple flowchart for computing a factorial N (N!)



https://en.wikipedia.org/wiki/Flowchart

Control of flow

- **Unconditional branches or jumps**
  - e.g., ill-famed *GOTO* of BASIC
  - not recommended as it leads to the "spaghetti code"!
- **Conditional execution**
  - executing a set of statements only if some conditions are met
  - *If –then – (else)*
- **Loops**
  - body of the loop is executed a specified number of times, or once for each of a collection of items, or until some condition is met, or indefinitely
    - Count-controlled loops: *for* loops in many languages
    - Condition-controlled loops: *while, until*
    - Collection-controlled loops:
      allow looping through all elements of a variable (e.g., an array), or all members of a set or collection
      e.g., *for, apply* or *lapply* in R

https://en.wikipedia.org/wiki/Control_flow

Conditional execution – examples in R and Python

if(*condition***)** *expression1* **else** *expression2*

- If condition evaluates to TRUE, expression1 is executed, otherwise expression2 is run.
- In R, complicated commands may be grouped together in braces:

R

```
x <- 6
y <- 0.5
if(x>2 & y<1){
    print(x)
    print(y)
}else{
    cat("Out of range\n")
}
```

Python

```
x = 6
y = 0.5
if x>2 and y<1:
    print(x)
    print(y)
else:
    print("Out of range")
```

Loop – examples in R and Python

for(*variable* **in** *expression1***)** *expression2*

- expression2 is a chunk of R code, usually grouped in braces to be executed repeatedly
- It is done exactly once for each of the values of the control variable, defined by expression1:

R

```
for(f in seq(1,10,by=2)){
    cat("Square root of",f,"is",sqrt(f),"\n")
}
```

Python

```
from numpy import sqrt
for f in range(1, 10, 2):
    print("Square root of", f, "is", sqrt(f))
```

Control of flow

- **Subroutines / procedures**
  - executing a set of distant statements
  - usually after their execution, the flow of control returns back
  - also known as: functions (especially if they return some results) or methods (in Object Oriented Programming, where they are associated with classes)
- **Unconditional halt**
  - prevents any further execution
  - often accompanied by an error message (in error handling)

Functions – examples in R and Python

function.name **<- function(***argument1, argument2, …***)** *expression*

- The `expression` is a chunk of R code, usually grouped in braces
- In order to avoid confusion, the last statement should be `return(var)`, where var is an expression or variable name giving the value(s) to be returned by the function

R

```
stdev <- function(x){
     z <- sqrt(sum((x-mean(x))^2)/length(x))
     return(z)
}
```

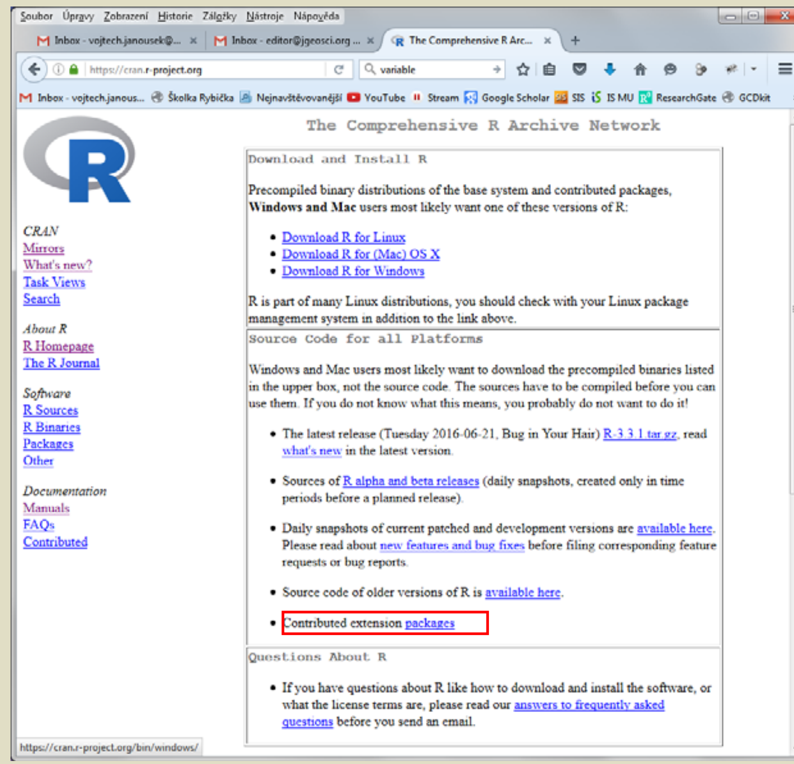
$$S = \sqrt{\frac{\sum_{i=1}^{n}\left(x_i - \bar{x}\right)^2}{n}}$$

Python

```
from numpy import sqrt, sum, mean
def stdev(x):
    z = sqrt(sum((x - mean(x))**2) / len(x))
    return z
```

Packages (R)

- **Packages (“libraries”)**
  - Collections of functions may be provided by external libraries
  - Frequently provide **“toolboxes”** related to a certain task/activity (e.g., R2HTML – output to web pages)
  - Mechanism for distribution of user-defined additions from the Internet community (e.g., CRAN)
  - Often may be **written in some other language** (e.g., calling a C or Fortran code)
  - This can be useful if speed of computation is critical



Scoping and namespaces

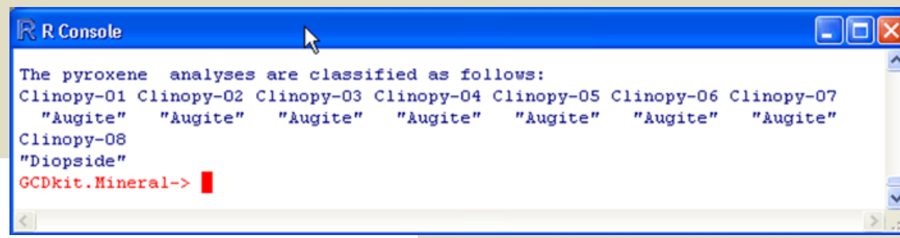
Variable / object types – general definition based on its lifetime

- **Global**
  (always known)
- **Local**
  (particular just to a part of the program, e.g. known only within some procedure)

Object-oriented programming (OOP)

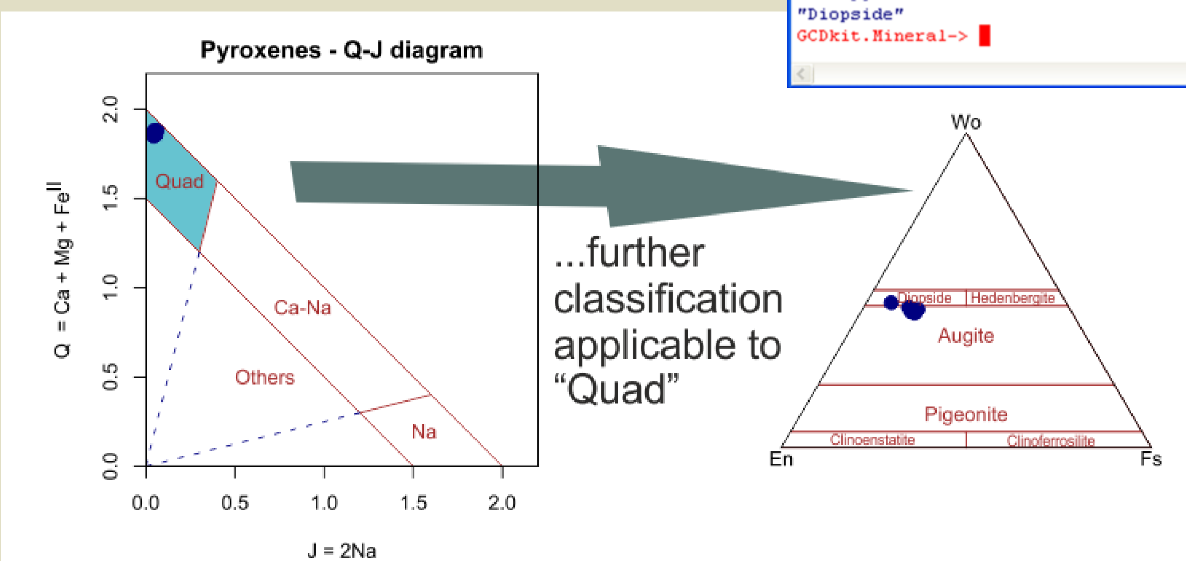
An example – R language (*GCDkit.Mineral*)

- each mineral (*feldspar*, *pyroxene*...) = a subclass of the class *mineral*
- method for formatted printing of the mineral class (for the generic function *print*)
- methods for recalculations to mineral formulae for each mineral species (a subclass)
- methods for IMA classification, based on a pre-defined sequence of binary or ternary plots...



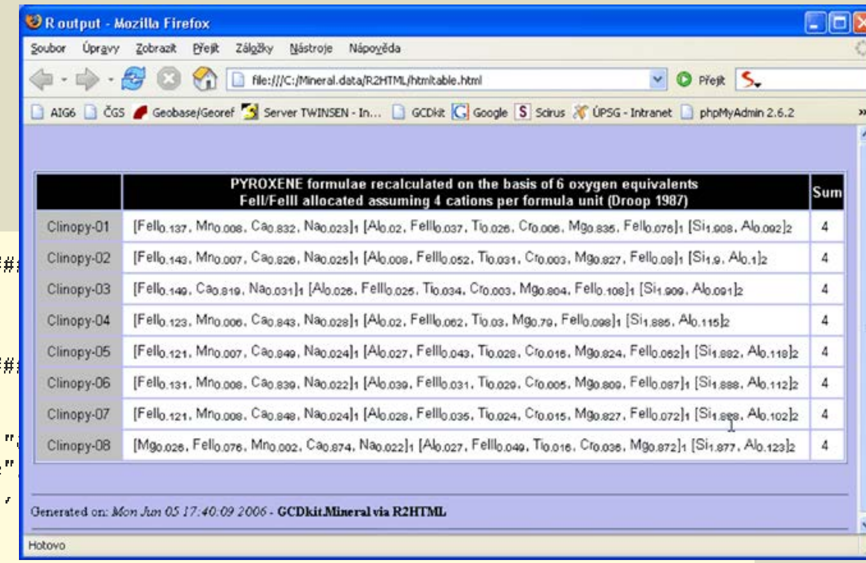
R Console

```
The pyroxene  analyses are classified as follows:
Clinopy-01 Clinopy-02 Clinopy-03 Clinopy-04 Clinopy-05 Clinopy-06 Clinopy-07
  "Augite"   "Augite"   "Augite"   "Augite"   "Augite"   "Augite"   "Augite"
Clinopy-08
"Diopside"
GCDkit.Mineral->
```



Object-oriented programming (OOP)

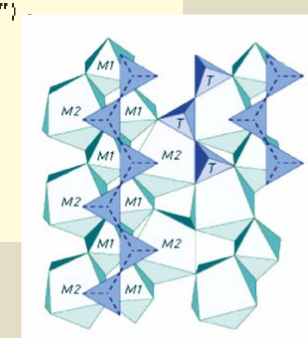
An example – R language (*GCDkit.Mineral*)



	PYROXENE formulae recalculated on the basis of 6 oxygen equivalents FeII/FeIII allocated assuming 4 cations per formula unit (Droop 1987)	Sum
Clinopy-01	$[FeII_{0.137}, Mn_{0.008}, Ca_{0.832}, Na_{0.023}]_1$ $[Al_{0.02}, FeIII_{0.037}, Ti_{0.026}, Cr_{0.006}, Mg_{0.835}, FeII_{0.076}]_1$ $[Si_{1.908}, Al_{0.092}]_2$	4
Clinopy-02	$[FeII_{0.143}, Mn_{0.007}, Ca_{0.826}, Na_{0.025}]_1$ $[Al_{0.008}, FeIII_{0.052}, Ti_{0.031}, Cr_{0.003}, Mg_{0.827}, FeII_{0.08}]_1$ $[Si_{1.9}, Al_{0.1}]_2$	4
Clinopy-03	$[FeII_{0.149}, Ca_{0.819}, Na_{0.031}]_1$ $[Al_{0.026}, FeIII_{0.025}, Ti_{0.034}, Cr_{0.003}, Mg_{0.804}, FeII_{0.108}]_1$ $[Si_{1.909}, Al_{0.091}]_2$	4
Clinopy-04	$[FeII_{0.123}, Mn_{0.006}, Ca_{0.843}, Na_{0.028}]_1$ $[Al_{0.02}, FeIII_{0.062}, Ti_{0.03}, Mg_{0.79}, FeII_{0.098}]_1$ $[Si_{1.885}, Al_{0.115}]_2$	4
Clinopy-05	$[FeII_{0.121}, Mn_{0.007}, Ca_{0.849}, Na_{0.024}]_1$ $[Al_{0.027}, FeIII_{0.043}, Ti_{0.028}, Cr_{0.016}, Mg_{0.824}, FeII_{0.062}]_1$ $[Si_{1.882}, Al_{0.118}]_2$	4
Clinopy-06	$[FeII_{0.131}, Mn_{0.008}, Ca_{0.839}, Na_{0.022}]_1$ $[Al_{0.039}, FeIII_{0.031}, Ti_{0.029}, Cr_{0.005}, Mg_{0.809}, FeII_{0.087}]_1$ $[Si_{1.888}, Al_{0.112}]_2$	4
Clinopy-07	$[FeII_{0.121}, Mn_{0.008}, Ca_{0.848}, Na_{0.024}]_1$ $[Al_{0.028}, FeIII_{0.035}, Ti_{0.024}, Cr_{0.015}, Mg_{0.827}, FeII_{0.072}]_1$ [Si [illegible], $Al_{0.102}]_2$	4
Clinopy-08	$[Mg_{0.026}, FeII_{0.076}, Mn_{0.002}, Ca_{0.874}, Na_{0.022}]_1$ $[Al_{0.027}, FeIII_{0.049}, Ti_{0.016}, Cr_{0.036}, Mg_{0.872}]_1$ $[Si_{1.877}, Al_{0.123}]_2$	4

Generated on: *Mon Jun 05 17:40:09 2006* - **GCDkit.Mineral via R2HTML**

```
#####################################################
#                                PYROXENE
#                           M2[1]M1[1]T[2]O[6]
#
#####################################################
setClass("pyroxene",representation(),contains="mineral",
    prototype(
        abbreviated=c("Px","Cpx","Opx","Di","En","Fs","Hd","
        full=c("pyroxene","Ca clinopyroxene","orthopyroxene",
            "jadeite","pidgeonite","wollastonite","acmite"),
        oxygens=6,
        cations=4,
        iron="Droop",
        # Site allocation according to Morimoto 1988
        atom.names=c("Si","Al","FeIII","Ti","Cr","V","Zr","Zn","Mg","FeII","Mn","Li","Ca","Na","K"),
        sites=list(T=(c("Si","Al","FeIII")),M1=c("Al","FeIII","Ti","Cr","V","Zr","Zn","Mg","FeII","Mn"),
            M2=c("Mg","FeII","Mn","Li","Ca","Na","K")),
        site.sums=c(2,1,NA),
        values.formulae="pyroxene.r",
        values.names=c("FeIII/Fetot","XMg","AlIV/AlVI","AlIV","AlVI"),
        end.member.formulae="pyroxene.end.r",
        end.member.names=c("Jd","Ac","CaTi","CaCr","CaFe","CaTs","Esc","Wo","En","Fs","Ac")
    )
)
```



Object-oriented programming (OOP)

- *objects* contain data in the form of *fields* (e.g., in R termed *slots*)
- the most popular object-oriented languages are class-based, i.e. individual objects are just instances of a given *class*
- the definition of each class includes:
  - initializing function, creating a new object, also setting its default values
  - implementation of a class behavior (*methods* = procedures associated with an object of the given class)

Inheritance

- new (sub-) classes may be defined based on other, more general, simpler ones

Polymorphism

- the functions and operators with the same name can mean different things depending on the class of the operand (e.g., in R *print, plot, summary…*)
- generic functions (used if no specific method is defined for the given class)

Encapsulation

- data and procedures belonging to a particular class are only available for that class

Human readability of the code

– The ease with which a human can comprehend the purpose, flow, and operation of source code

– It may have little to do with the actual code speed/effectivity!

– Human readability can be improved by:

- Using different **indentation styles** (whitespace)
- Extensive use of **comments**, writing detailed **documentation**
- **Decomposition**
  breaking a complex problem into parts that are easier to understand, program and maintain
- **Structured (= modular) programming** which employs:
- block structures
  e.g., in R these are grouped by braces, { }
- subroutines/functions
- conditionals – *if else*
- *for* and *while* loops

https://en.wikipedia.org/wiki/Computer_programming

- Adopting **naming conventions** for objects (variables, functions, classes…)
- Strict and consistent use of naming conventions and structured programming techniques ideally lead to **self-documenting code**

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