

BIOC0023 – A (shortened) introduction to computing

Andrew C.R. Martin
University College London

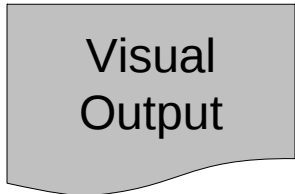
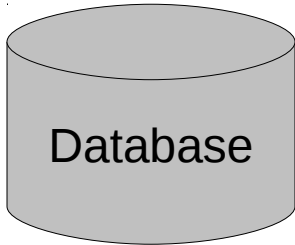
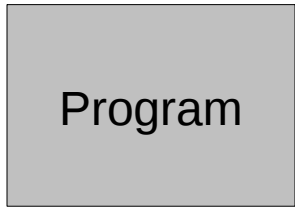
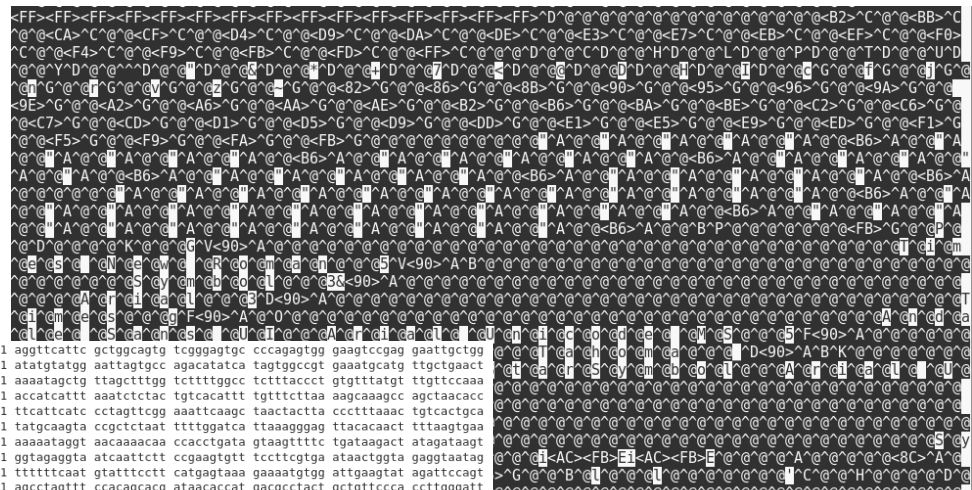
Aims and Objectives

To introduce some fundamentals of:

- **Computing concepts**
- **Operating systems**
- **Databases**
- **Algorithms**
- **Programming**
- **Using the command line**

Computing concepts

Computing concepts

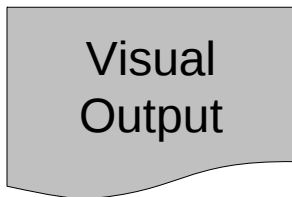
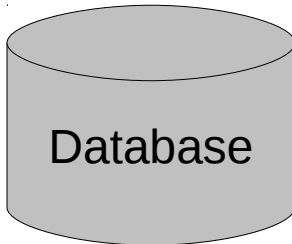
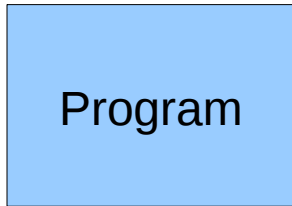
```

1 aggttcattc gctgcagtg tcggagatgc cccaagtggt gaagtcgag gaattgctgg
61 atatgtatgg aattagtgcc agacataca tagtgcgctt gaaatcgatg ttgctgaact
121 aaaatgctgt ttatctttgg tcttttggcc tctttaccct ggtttatgat ttgttccaaa
181 acctcattt aaatctctac tgtcacattt tgtttcttaa aagcaaaagc agctaacacc
241 ttcatctatc cctagtctgg aaattcaagc taactactta ccccttaaac tgtcaactgca
301 tatgacaagt ccgtcttaat ttttggatca ttaaaggagc ttacacaact tttaatgtaa
361 aaaaataggt acaaaaacaa ccactcgata gtaagttttc tgataagact atagataagt
421 ggtagaggta atcaattctt ccgaagtttt tccctctgta atactcggta gaggtaatag
481 tttttcaat gtatttctct catgagtaaa gaaaattggtg attgaagat agttccaggt
541 agcctagttt ccacagcagc ataacaccat gacgcttact gctgtctcca ccttggagat
601 ctgtgtgctg ccatccccc tgacgtgccc ctgaaatccc ctctctgttt tgctccatc
661 tccctccagc ttgpagagcg tgcaggcagc cagcgaagcg ttgttagat gtcctgtgct
721 gctgtgatg agagcctcca cactrtacta ttcaantraa tttaattaaa acatttcaaa
781 acagctgctt ttattcagca cgtg ATOM 120 C GLU L 17 -12.869 -9.053 17.387 1.00 29.00 C
841 taataaagga aagagctttt atccc ATOM 121 0 GLU L 17 -12.097 -8.093 17.476 1.00 27.63 0
901 acctggpaaa gaataatggg ctgci ATOM 122 CB GLU L 17 -12.718 -10.348 15.276 1.00 31.42 C
961 aaaagctgtc cctgagctga cgccc ATOM 123 CG GLU L 17 -13.476 -11.182 14.257 1.00 38.05 C
1021 gaggccagcg gttgtgctc agcgc ATOM 124 CD GLU L 17 -12.575 -12.170 13.538 1.00 41.19 C
1081 gatcacctga ggtcaggagt tcaaa ATOM 125 OE1 GLU L 17 -11.786 -12.864 14.217 1.00 43.88 0
1141 ctaaaaagga caaaaattag ccagi ATOM 126 OE2 GLU L 17 -12.660 -12.265 12.295 1.00 45.79 0
1201 gaggctgag caggagaatt gtttt ATOM 127 N LYS L 18 -13.1D G6PD HUMAN Reviewed; 515 AA.
1261 ctgccattgt accgcagcct aggai ATOM 128 CA LYS L 18 -12. AC P11413; D3DMX9; Q16080; Q16765; O81U70; O81U88; O81UA6; O96P02;
1321 gaagtatga tctagaatca aagtt ATOM 129 C LYS L 18 -11. DT 01-OCT-1989, integrated into UniProtKB/Swiss-Prot.
1381 agatttaaaa tctactagta tgg ATOM 130 0 LYS L 18 -10. DT 23-JAN-2007, sequence version 4.
1441 gttttgagac aggttctcac tatg ATOM 131 CB LYS L 18 -13. DT 09-DEC-2015, entry version 212.
1501 atcttcacgc ctggaccctc caagi ATOM 132 CG LYS L 18 -12. DE ReName: Full+Glucose-6-phosphate 1-dehydrogenase;
Short+G6PD;
Ec1.1.1.49;
Name=G6PD;
13. OS Homo sapiens (Human).
10. OC Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi;
Mammalia; Eutheria; Euarchontoglires; Primates; Haplorhini;
Carnivora; Hominoidea; Homo.
-8. OX NCBI TaxID=9606;
-8. RN [1]
-7. RP NUCLEOTIDE SEQUENCE [MRNA] (ISOFORM SHORT).
PubMed=3513519; DOI=10.1093/nar/14.6.2511;
-6. RA Persico M.G., Viglietto G., Martini G., Toniolo D., Poanessa G.,
Moscatelli G., Dono R., Vulliamy T.J., Luzzatto L., D'Urso M.;
-7. RT "Isolation of human glucose-6-phosphate dehydrogenase (G6PD) cDNA
clones: primary structure of the protein and unusual 5' non-coding
region."
RL Nucleic Acids Res. 14:2511-2522(1986).
RN [2]
RP NUCLEOTIDE SEQUENCE [GENOMIC DNA].
PubMed=2428611;
RA Martini G., Toniolo D., Vulliamy T., Luzzatto L., Dono R.,
RA Viglietto G., Poanessa G., D'Urso M., Persico M.G.;
RT "Structural analysis of the X-linked gene encoding human glucose 6-
phosphate dehydrogenase.;"
RL EMBO J. 5:1849-1855(1986).
RN [3]
RP NUCLEOTIDE SEQUENCE [MRNA] (ISOFORM SHORT), PARTIAL NUCLEOTIDE
SEQUENCE [MRNA] (ISOFORM LONG), AND VARIANTS NSHA MET-68 AND ASP-126.
PubMed=2636867; DOI=10.1073/pnas.85.11.3951;
RX Hirono A., Boutler E.;
RT "Molecular cloning and nucleotide sequence of cDNA for human glucose-
6-phosphate dehydrogenase variant A1.;"
RL Proc. Natl. Acad. Sci. U.S.A. 85:3951-3954(1988).

```



Computing concepts



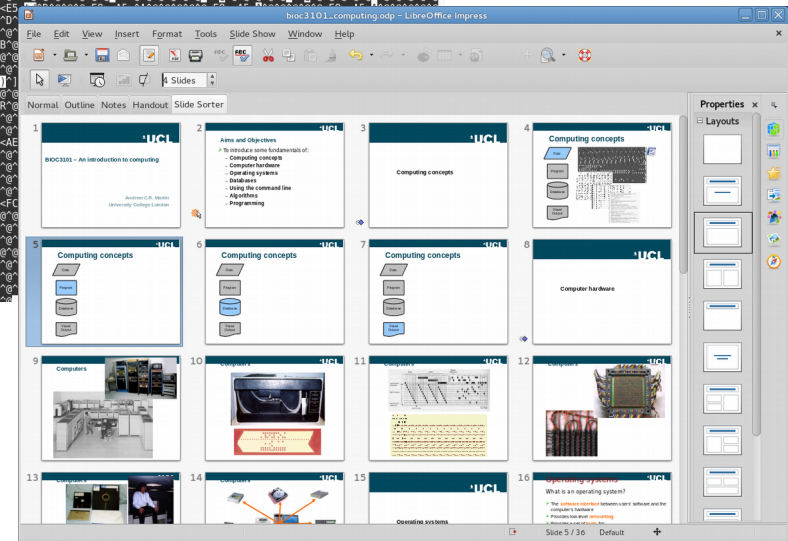
```

/* Read PDB file
if((wpdb = blReadWholePDBAtoms(in)) == NULL)|| (wpdb->pdb==NULL))
{
    fprintf(stderr,"Error: Unable to read atoms from input file%s\n",
            ((gLabel[0])?" Label: ":""),
            ((gLabel[0])?gLabel:""));
    return(1);
}
wpdb =wpdb->pdb;

if(UseSEQRES)
{
    /* Read MODRES and SEQRES records
modres = blGetModresWholePDB(wpdb);
seqres = blGetSeqresAsStringWholePDB(wpdb, seqchains, modres,
doNucleic);
}

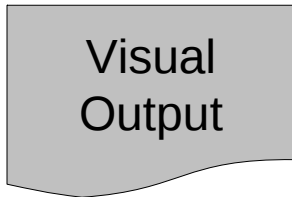
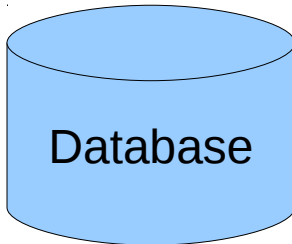
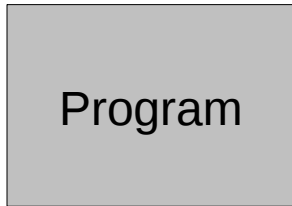
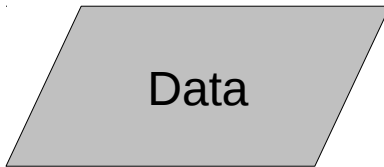
/* Extract sequence from PDB linked list
if((atomchains = blGetPDBChains(wpdb, seqchains)) == NULL)
{
    fprintf(stderr,"Error: No atom chains found\n");
    return(1);
}

/* Convert PDB linked list
if(SkipX)
{
    if(doNucleic)
    {
        if((sequence = blPDB2Seq(wpdb, seqchains, atomchains, doNucleic)) == NULL)
        {
            fprintf(stderr,"Error: No sequence found\n");
            return(1);
        }
    }
}
    
```



The screenshot shows the LibreOffice Impress application window. The title bar reads 'bioc3101.computing.odp - LibreOffice Impress'. The menu bar includes File, Edit, View, Insert, Format, Tools, Slide Show, Window, and Help. Below the menu bar is a toolbar with various icons. The main area displays a 'Slide Sorter' view with 16 slides arranged in a grid. The first slide is titled 'BIOC3101 - An introduction to computing' and lists topics: 'Areas and sub-systems', 'To introduce some fundamentals of', 'Computing hardware', 'Computing software', 'Databases', 'Operating systems', 'Algorithms', and 'Programming'. The current slide (Slide 5) is 'Computing concepts' and features a diagram of a computer system with components like 'Data', 'Program', 'Database', and 'Visual Output'. Other slides include 'Computer hardware', 'Computers', 'Operating systems', and 'What is a operating system?'. The status bar at the bottom indicates 'Slide 5 / 36 Default'.

Computing concepts



```
CREATE TABLE data_source_type (
  data_source_type_id serial PRIMARY KEY,
  data_source_type_name varchar(100) NOT NULL UNIQUE check ( data_source_type_name <> '' ),
  display_name varchar(100) NOT NULL UNIQUE check ( display_name <> '' ),
  display_order integer NOT NULL
);

CREATE TABLE chain_type (
  chain_type_id serial PRIMARY KEY,
  chain_type_name varchar(100) NOT NULL UNIQUE check ( chain_type_name <> '' ),
  higher_chain_type_id integer,
  display_name varchar(100) NOT NULL UNIQUE check ( display_name <> '' ),
  receptor_type_particle varchar(100) NOT NULL UNIQUE check ( receptor_type_particle <> '' ),
  display_order integer NOT NULL,

  FOREIGN KEY(higher_chain_type_id) REFERENCES chain_type(chain_type_id)
);

CREATE TABLE human_subgroup (
  human_subgroup_id serial PRIMARY KEY,
  human_subgroup_name varchar(100) NOT NULL UNIQUE check ( human_subgroup_name <> '' ),
  chain_type_id integer NOT NULL,
  display_name varchar(100) NOT NULL UNIQUE check ( display_name <> '' ),
  display_order integer NOT NULL,

  FOREIGN KEY(chain_type_id) REFERENCES chain_type(chain_type_id)
);

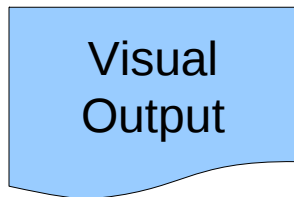
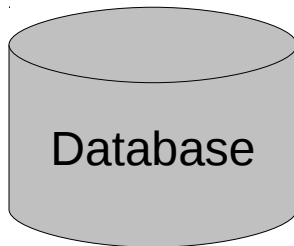
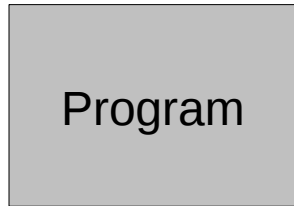
CREATE TABLE segment_type (
  segment_type_id serial PRIMARY KEY,
  display_name varchar(100) NOT NULL UNIQUE check ( display_name <> '' ),
  display_order integer NOT NULL
);

CREATE TABLE region_type (
  region_type_id serial PRIMARY KEY,
  region_type_name varchar(100) NOT NULL UNIQUE check ( region_type_name <> '' ),
  chain_type_id integer NOT NULL,
  display_name varchar(100) NOT NULL UNIQUE check ( display_name <> '' ),
  display_order integer NOT NULL,

  FOREIGN KEY(chain_type_id) REFERENCES chain_type(chain_type_id)
);
```

The screenshot shows the UniProtKB web interface for the protein P11413 (G6PD_HUMAN). At the top, there is a search bar with 'UniProtKB' and a search button. Below the search bar, there are navigation options: BLAST, Align, and Retrieve/D mapping. The main header of the page is 'UniProtKB - P11413 (G6PD_HUMAN)'. On the left side, there are tabs for Protein, Gene, and Organism. The 'Protein' tab is selected, showing 'Glucose-6-phosphate 1-dehydrogenase' and 'G6PD'. Below this, there is a 'Status' section showing 'Reviewed - Annotation score: 100% - Experimental evidence at protein level'. The 'Display' section has a dropdown menu set to 'None'. The 'Function' section is expanded, showing a detailed description of the enzyme's role in the oxidative pentose-phosphate pathway. Below the function, there are sections for 'Catalytic activity', 'Kinetics', and 'Pathway'. The 'Catalytic activity' section shows the reaction: D-glucose 6-phosphate + NADP⁺ = 6-phospho-D-glucono-1,5-lactone + NADPH. The 'Kinetics' section shows $K_M = 7.07 \mu M$ for NADP and $K_M = 52 \mu M$ for glucose 6-phosphate. The 'Pathway' section shows that the protein is involved in the 'pentose phosphate pathway' and 'step 1' of the subpathway that synthesizes D-ribulose 5-phosphate from D-glucose 6-phosphate (oxidative stage).

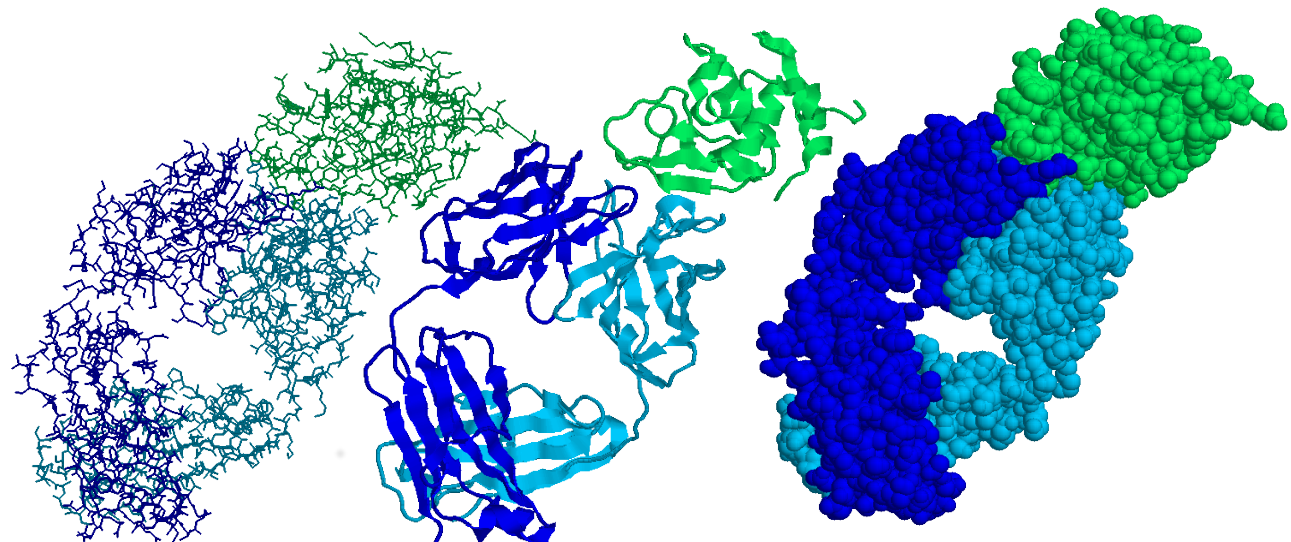
Computing concepts



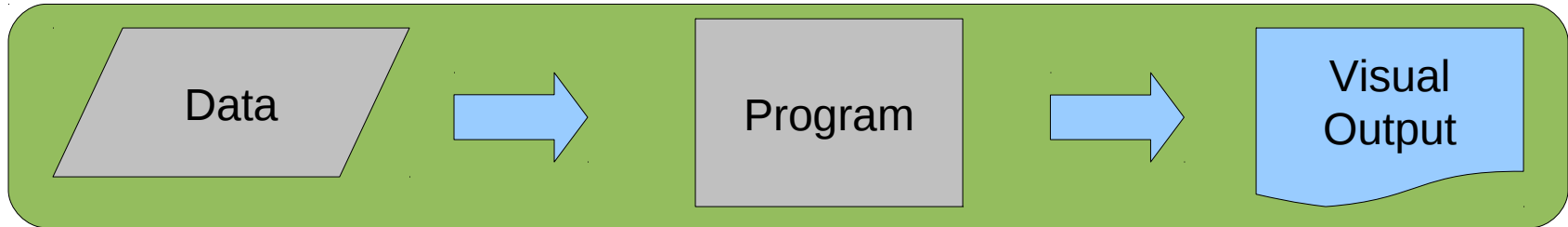
All/None

<input type="checkbox"/>	id1b1.L	S	A	S	S	V	N	Y	M	Y	A	C	R	E	F	G	H	I	K	L	M	N	P	T	R	S	T	V	W	Y	
<input type="checkbox"/>	id1a.L	S	A	S	S	T	N	Y	M	Y	A	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y	
<input type="checkbox"/>	id2b1.L	S	A	S	S	T	C	N	Y	M	T	A	C	D	E	E	G	H	I	K	L	M	N	P	-	R	S	T	C	W	Y
<input type="checkbox"/>	id2a.L	S	A	S	S	S	C	N	Y	M	T	L	C	D	E	H	G	H	I	K	L	M	N	P	-	R	S	T	C	W	Y
<input type="checkbox"/>	id2a1.L	S	A	S	S	S	C	N	Y	M	T	L	C	D	E	H	G	H	I	K	L	M	N	P	Q	R	S	T	C	W	Y
<input type="checkbox"/>	id1.L	S	A	S	S	V	N	Y	M	Y	A	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y	
<input type="checkbox"/>	id1b.L	S	A	S	S	V	N	Y	M	Y	A	C	R	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y	
<input type="checkbox"/>	id1a1.L	S	A	S	S	T	N	Y	M	Y	L	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y	
<input type="checkbox"/>	id2.L	S	A	S	S	S	C	N	Y	M	T	A	C	D	E	H	G	H	I	K	L	M	N	P	-	R	S	T	C	W	Y
<input type="checkbox"/>	id2b.L	S	A	S	S	T	C	N	Y	M	T	A	C	D	E	H	G	H	I	K	L	M	N	P	-	R	S	T	C	W	Y
Consensus		S	A	S	S	S	C	N	Y	M	T	A	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	C	W	Y

Sort Region:



Computing concepts



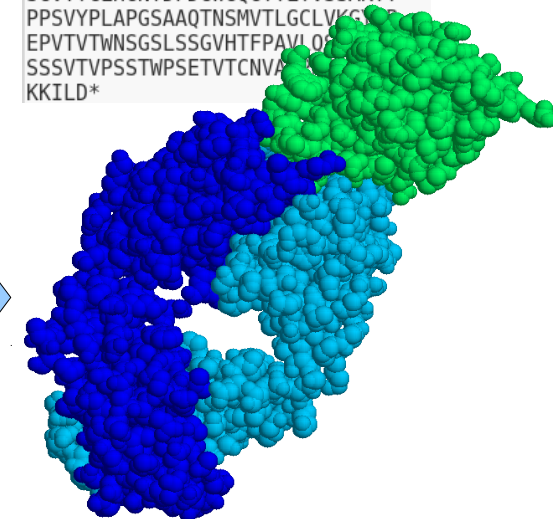
ATOM	120	C	GLU	L	17	-12.869	-9.053	17.387	1.00	29.00	C
ATOM	121	O	GLU	L	17	-12.097	-8.093	17.476	1.00	27.63	O
ATOM	122	CB	GLU	L	17	-12.718	-10.348	15.276	1.00	31.42	C
ATOM	123	CG	GLU	L	17	-13.476	-11.182	14.257	1.00	38.05	C
ATOM	124	CD	GLU	L	17	-12.575	-12.170	13.538	1.00	41.19	C
ATOM	125	OE1	GLU	L	17	-11.786	-12.864	14.217	1.00	43.88	O
ATOM	126	OE2	GLU	L	17	-12.660	-12.265	12.295	1.00	45.79	O
ATOM	127	N	LYS	L	18	-13.131	-9.865	18.403	1.00	27.62	N
ATOM	128	CA	LYS	L	18	-12.493	-9.684	19.695	1.00	25.99	C
ATOM	129	C	LYS	L	18	-11.113	-10.322	19.622	1.00	25.02	C
ATOM	130	O	LYS	L	18	-10.951	-11.410	19.072	1.00	25.02	O
ATOM	131	CB	LYS	L	18	-13.314	-10.351	20.794	1.00	28.03	C
ATOM	132	CG	LYS	L	18	-12.714	-10.191	22.176	1.00	28.69	C
ATOM	133	CD	LYS	L	18	-13.561	-10.879	23.234	1.00	31.64	C
ATOM	134	CE	LYS	L	18	-12.901	-10.773	24.598	1.00	33.25	C
ATOM	135	NZ	LYS	L	18	-13.706	-11.408	25.679	1.00	36.75	N
ATOM	136	N	VAL	L	19	-10.118	-9.643	20.178	1.00	23.61	N
ATOM	137	CA	VAL	L	19	-8.756	-10.152	20.155	1.00	22.78	C
ATOM	138	C	VAL	L	19	-8.168	-10.222	21.553	1.00	21.59	C
ATOM	139	O	VAL	L	19	-8.325	-9.300	22.347	1.00	21.97	O
ATOM	140	CB	VAL	L	19	-7.845	-9.259	19.292	1.00	22.79	C
ATOM	141	CG1	VAL	L	19	-6.398	-9.696	19.441	1.00	22.72	C
ATOM	142	CG2	VAL	L	19	-8.278	-9.336	17.832	1.00	24.05	C
ATOM	143	N	THR	L	20	-7.486	-11.321	21.846	1.00	22.21	N
ATOM	144	CA	THR	L	20	-6.865	-11.500	23.145	1.00	22.76	C

pdb2pir

```

>P1;PDBPIR
Sequence extracted from PDB file
MDIVLTQSPAIMASASPGEKVTMTCSASSSV
NYMYWYQQKSGTSPKRWIYDTSKLAGVVPV
RFSGSGSGTSYSLTISSMETEDAATYYCQQ
WGRNPTFGGGTKLEIKRADAAPTVISIFPPS
SEQLTSGGASVVCFLNNFYPKDINVKWKID
GSERQNGVLNSWTDQDQSKDSTYSMSSTLTL
TKDEYERHNSYTCETHKTSTSPIVKSFNR
N*
EVQLQQSGAELMKPGASVKISCKASGYTFS
DYWIEWVKQRPGHGLEWIGIEILPGSGSTNY
HERFKGKATFTADTSSSTAYMQLNSLTSED
SGVYYCLHGNYDFDGGWGQTTTLTVSSAKTT
PPSVYPLAPGSAAQTNMVTLGCLVKIGYSP
EPVTVTWNSSGLSSGVHFTPAVLIQD
SSSVTVPSSTWVPEVTVCNVA
KKILD*
  
```

RASMOL



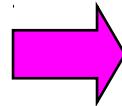
Operating systems

Operating Systems

- The **software interface** between users' software and the computer's hardware
- Provides low-level **networking**
- Provides a set of **tools** for:
 - file handling
 - user handling and security (e.g. passwords)
- May provide a **graphical user interface (GUI)**
- May include other non-essential **bundled tools**

Operating Systems

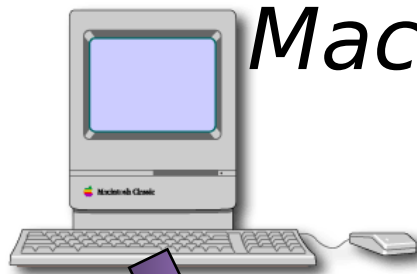
- VMS (Dec)
- VME (ICL)
- CP/M (PCs)
- PRIMOS (Prime)
- MS-DOS (PCs)
- OS/2 (PCs)
- AmigaDOS (CBM)
- Unix (Various)
- MacOS (Apple)



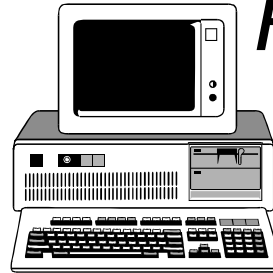
- Windows (PCs)
- Unix/Linux (Various)
- MacOS (Apple)

Operating Systems

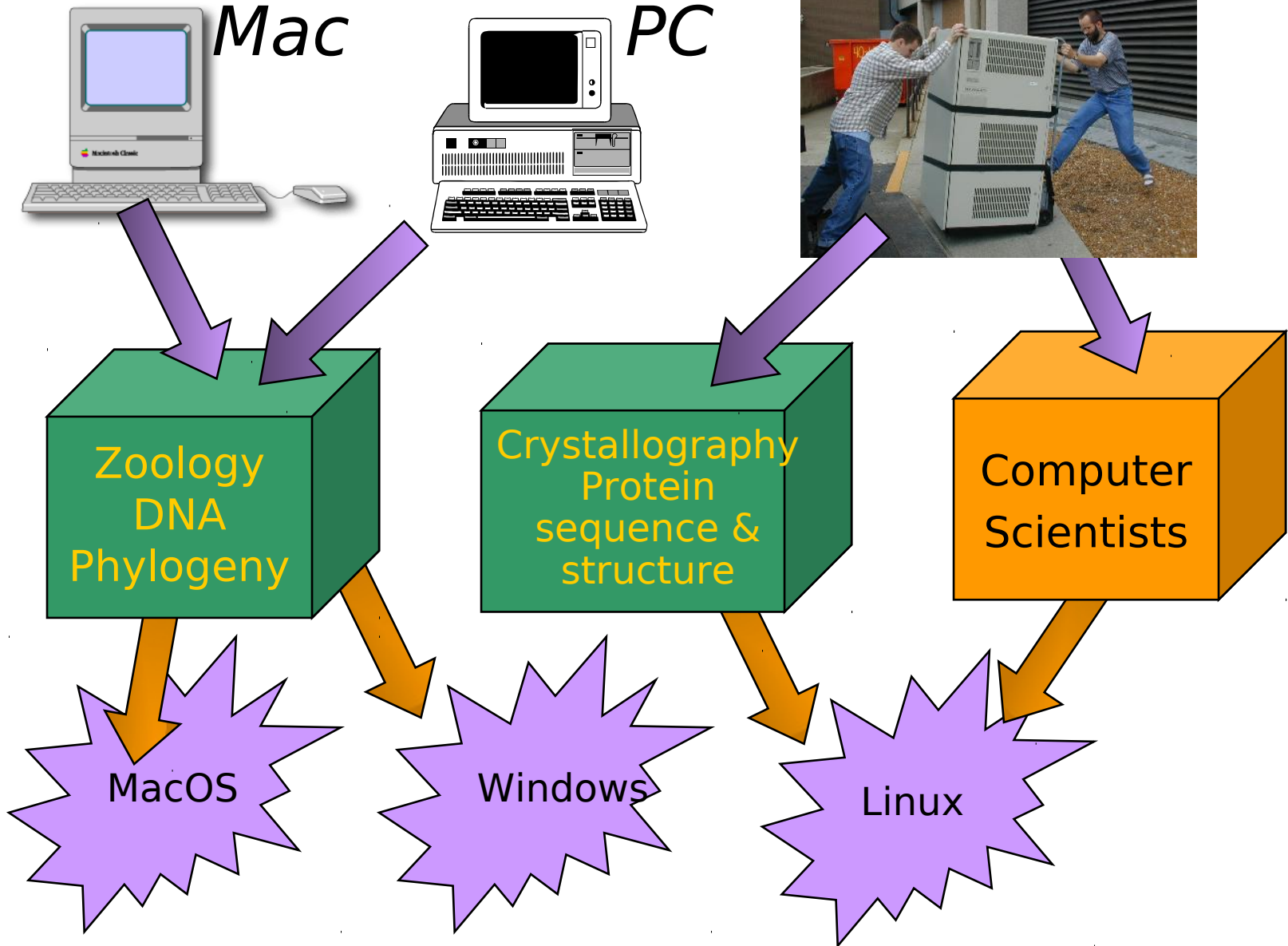
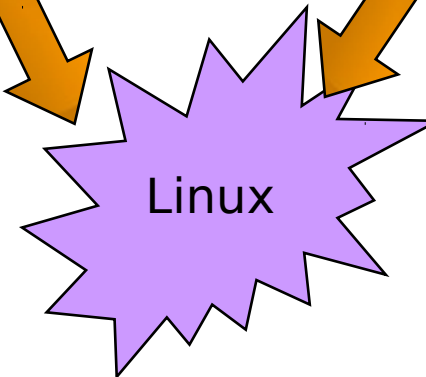
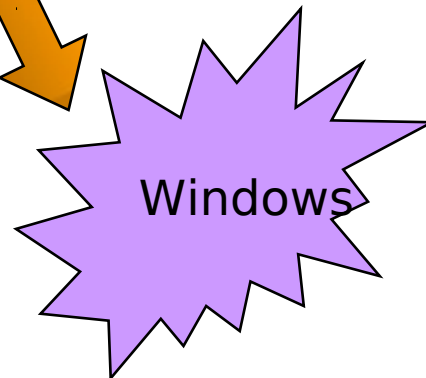
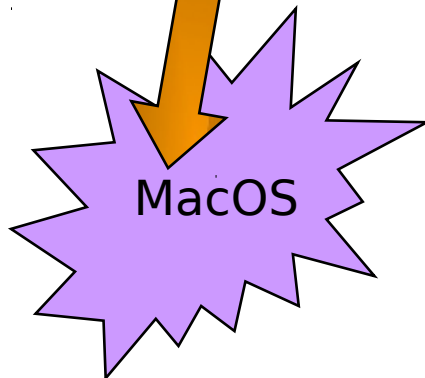
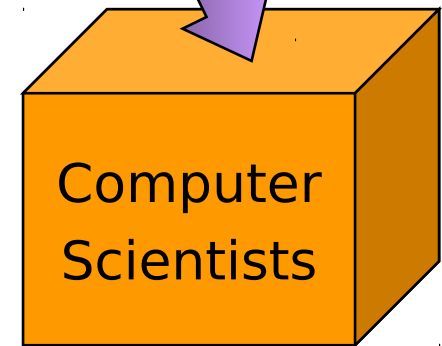
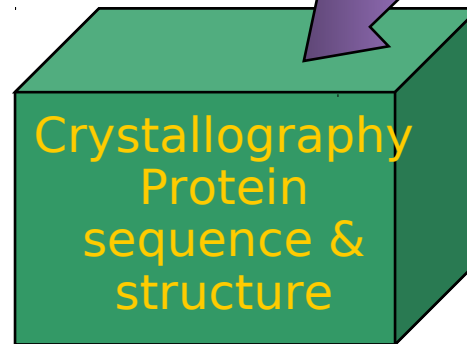
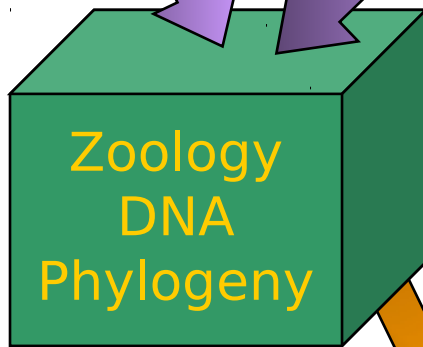
Mini/Mainframe



Mac



PC



Databases

Databases and databanks

➤ Databank

- A collection of data (normally in simple text files) without an associated query tool
- Query tools may be written as separate applications

➤ Database

- A structured collection of data with some tool enabling it to be 'queried'

Relational databases

- Microsoft Access
- SQL Server
- Oracle
- Sybase
- MySQL
- PostgreSQL

Relational databases

- Data are separated into **tables** or **relations**
- Good **database design** requires
 - careful thought and planning
 - normalization
- Maintains **data integrity**

SQL - Structured Query Language

- **'Standard'** database query language
 - Unfortunately most databases extend or deviate from the standard

- Provides 4 types of command:
 - **Schema** creation
 - Data **insertion**
 - Data **extraction**
 - Database **management**

Algorithms

Algorithms

“A process or set of rules to be followed in calculations or other problem-solving operations, especially by a computer.”

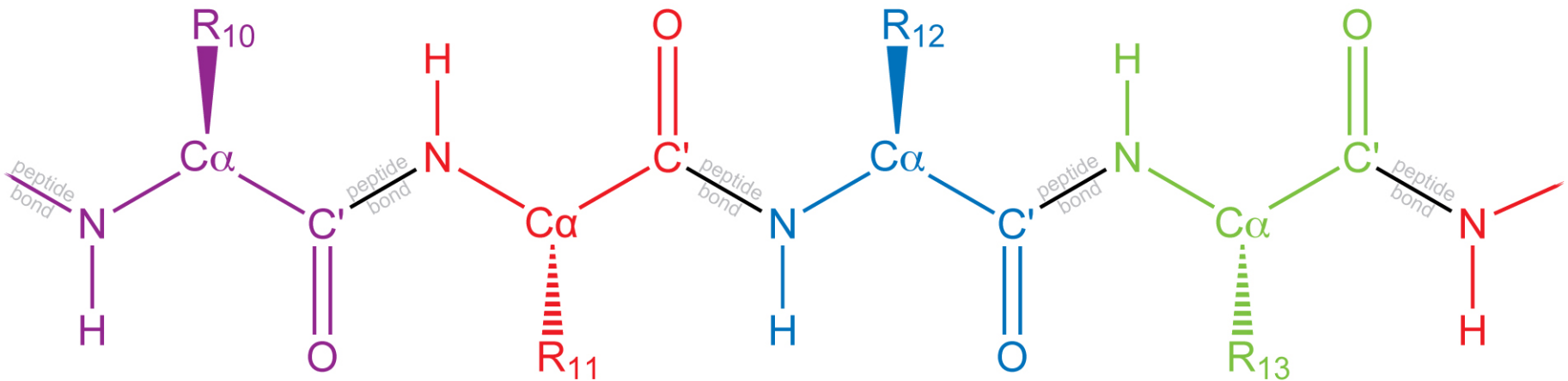
A **complete and precise set of steps** that will solve a problem and achieve an identical result whenever given the same set of data to a defined level of accuracy.

- **Ordered steps**
- **Repeatable**
- **Known/defined accuracy**

Algorithms

Suppose we wish to count the amino acids in a PDB file...

Count the C-alpha (CA) atoms



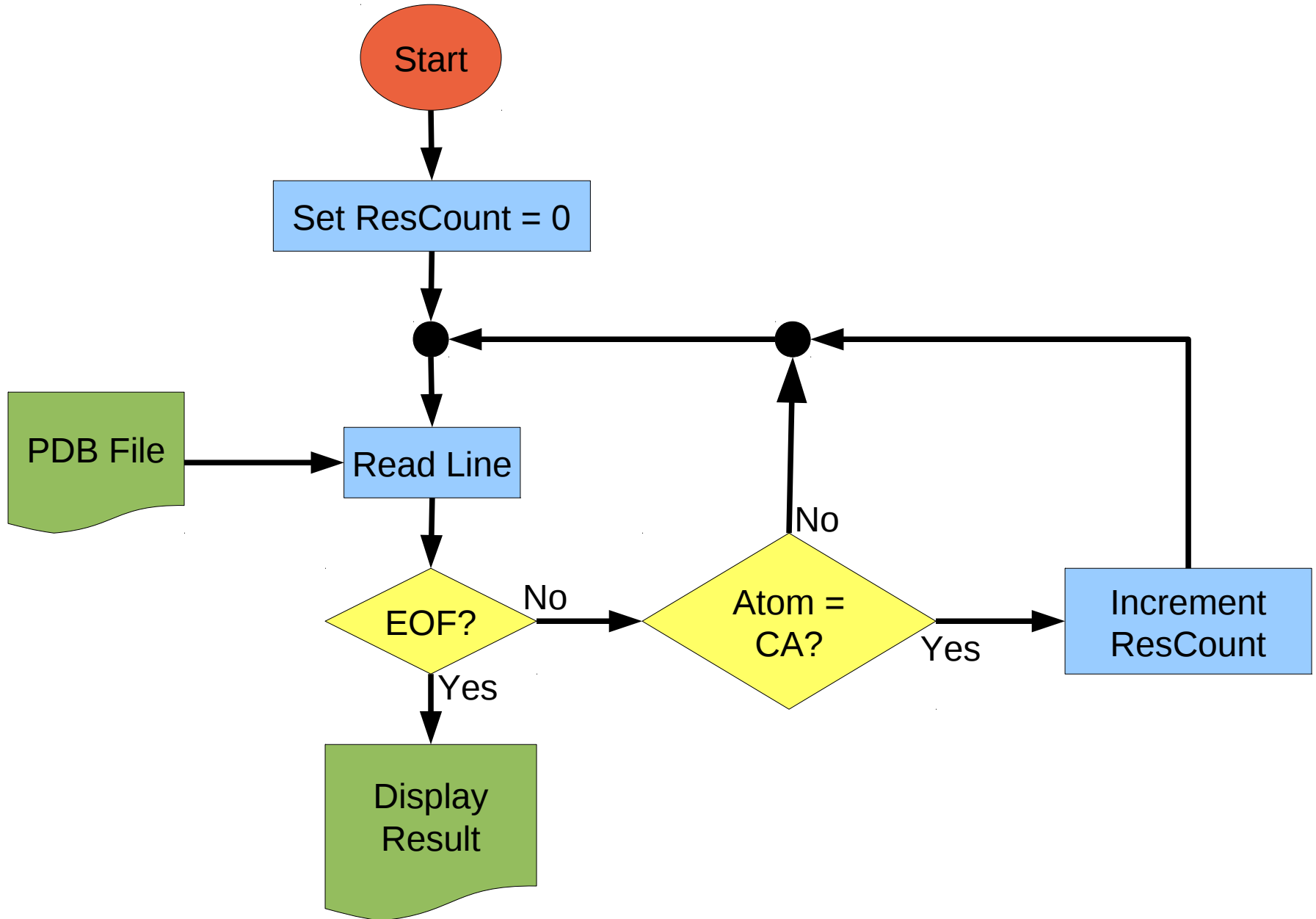
Loren Williams

Image from:
ww2.chemistry.gatech.edu/~lw26/structure/protein/peptide_bond/

Algorithms

Count the CA atoms

ATOM	412	N	LYS	L	53	-3.744	0.441	32.828	1.00	19.24	N
ATOM	413	CA	LYS	L	53	-3.918	1.859	32.529	1.00	21.00	C
ATOM	414	C	LYS	L	53	-3.602	2.152	31.066	1.00	19.26	C
ATOM	415	O	LYS	L	53	-2.544	1.771	30.559	1.00	19.24	O
ATOM	416	CB	LYS	L	53	-3.005	2.700	33.430	1.00	22.69	C
ATOM	417	CG	LYS	L	53	-3.163	2.411	34.918	1.00	27.89	C
ATOM	418	CD	LYS	L	53	-4.592	2.607	35.383	1.00	31.37	C
ATOM	419	CE	LYS	L	53	-4.727	2.311	36.869	1.00	34.46	C
ATOM	420	NZ	LYS	L	53	-6.149	2.369	37.331	1.00	34.97	N
ATOM	421	N	LEU	L	54	-4.514	2.835	30.382	1.00	19.88	N
ATOM	422	CA	LEU	L	54	-4.303	3.155	28.975	1.00	18.71	C
ATOM	423	C	LEU	L	54	-3.428	4.390	28.776	1.00	21.13	C
ATOM	424	O	LEU	L	54	-3.642	5.427	29.410	1.00	20.98	O
ATOM	425	CB	LEU	L	54	-5.646	3.368	28.271	1.00	20.67	C
ATOM	426	CG	LEU	L	54	-6.632	2.192	28.234	1.00	22.27	C
ATOM	427	CD1	LEU	L	54	-7.786	2.553	27.308	1.00	24.52	C
ATOM	428	CD2	LEU	L	54	-5.938	0.930	27.745	1.00	24.94	C
ATOM	429	N	ALA	L	55	-2.439	4.276	27.895	1.00	20.95	N
ATOM	430	CA	ALA	L	55	-1.550	5.397	27.602	1.00	20.98	C
ATOM	431	C	ALA	L	55	-2.332	6.453	26.820	1.00	22.37	C
ATOM	432	O	ALA	L	55	-3.423	6.179	26.311	1.00	20.12	O
ATOM	433	CB	ALA	L	55	-0.355	4.916	26.792	1.00	20.40	C
ATOM	434	N	SER	L	56	-1.779	7.657	26.718	1.00	25.32	N
ATOM	435	CA	SER	L	56	-2.468	8.731	26.009	1.00	27.06	C
ATOM	436	C	SER	L	56	-2.741	8.390	24.547	1.00	25.53	C
ATOM	437	O	SER	L	56	-1.869	7.888	23.833	1.00	26.22	O
ATOM	438	CB	SER	L	56	-1.671	10.038	26.099	1.00	29.91	C
ATOM	439	OG	SER	L	56	-0.396	9.914	25.494	1.00	35.66	O
ATOM	440	N	GLY	L	57	-3.972	8.652	24.117	1.00	25.76	N
ATOM	441	CA	GLY	L	57	-4.359	8.380	22.748	1.00	24.53	C
ATOM	442	C	GLY	L	57	-4.862	6.970	22.498	1.00	24.68	C
ATOM	443	O	GLY	L	57	-5.416	6.694	21.437	1.00	25.32	O
ATOM	444	N	VAL	L	58	-4.684	6.075	23.464	1.00	22.98	N
ATOM	445	CA	VAL	L	58	-5.130	4.693	23.286	1.00	22.67	C
ATOM	446	C	VAL	L	58	-6.646	4.581	23.452	1.00	23.27	C
ATOM	447	O	VAL	L	58	-7.192	4.959	24.490	1.00	22.54	O
ATOM	448	CB	VAL	L	58	-4.426	3.758	24.290	1.00	21.70	C
ATOM	449	CG1	VAL	L	58	-4.874	2.315	24.068	1.00	19.47	C
ATOM	450	CG2	VAL	L	58	-2.918	3.878	24.129	1.00	20.49	C

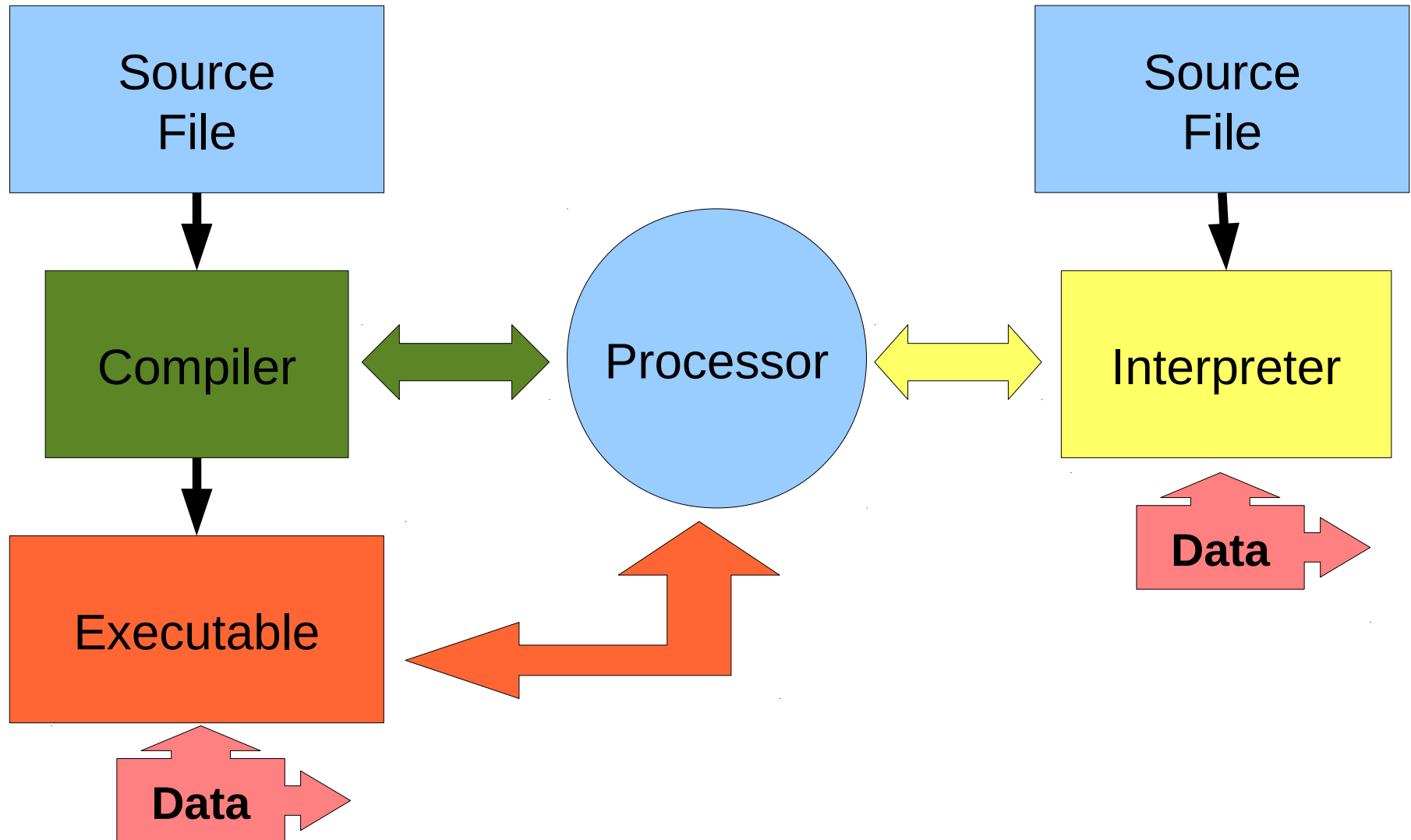


Programming

Programming languages

- Rarely write directly in instructions understood by a computer
- Use a **high-level language**
- Many such languages:
 - **C**
 - **Perl**
 - **C++**
 - **Java**
 - Smalltalk
 - **Python**
 - Forth
 - BASIC
 - **FORTRAN**
 - Modula-II
 - Simula
 - Prolog
 - BCPL
 - **JavaScript**
 - Pascal
 - AWK
 - LISP
 - Cobol

Language Categories



General Purpose Languages - Python

General Purpose / JIT/Part-Compiled / OO

- Design emphasizes code readability; concise syntax.
- Comprehensive standard library, plus maths and scientific and BioPython libraries.

Variables

Scalar variables

```
a = 5  
a = a + 1  
print (a)  
b = 'Hello world'
```

Variables

Lists / Arrays (vectors)

```
position = [5.4, 2.7, 9.5]
print (position[1])
position[2] = 3.6
```

Variables

Dictionaries / Hashes

```
position          = {}  
position['x']    = 5.4  
position['y']    = 2.7  
position['z']    = 9.5
```

Control statements

if:

```
x = -6
if x > 0:
    print "Positive"
elif x == 0:
    print "zero"
else:
    print "negative"
```

Comparisons:

< <= == >= > !=

Control statements

while:

```
x = 5
while x > 0:
    print x
    x = x - 1
```

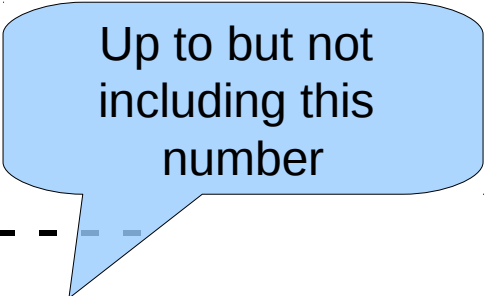
Control statements

for:

```
x = [100, 200, 300]
```

```
for i in x:
```

```
    print i
```



Up to but not including this number

```
for i in range(0, 100):
```

```
    print i
```

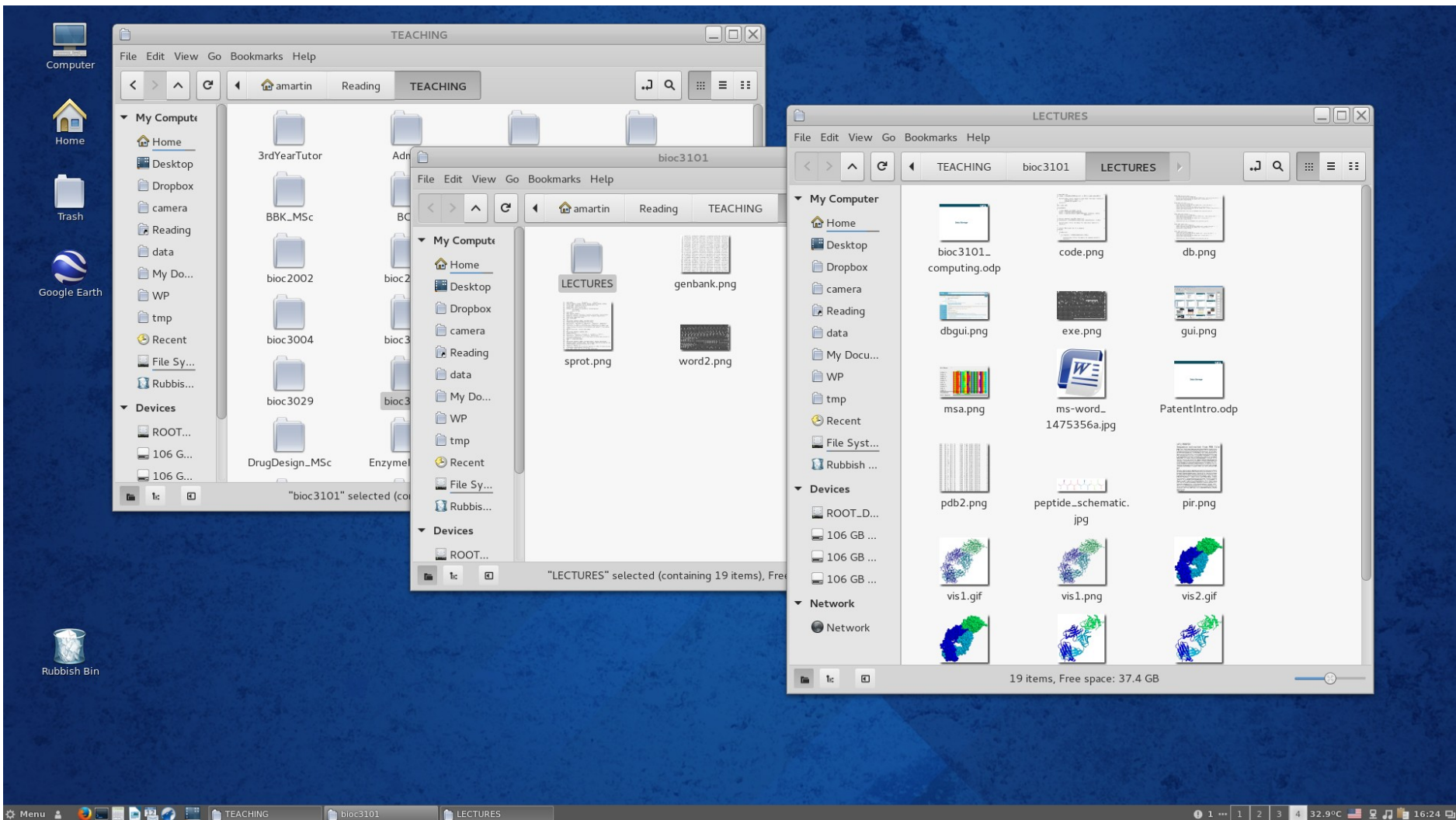
```
x = [100, 200, 300]
```

```
for i in range(3):
```

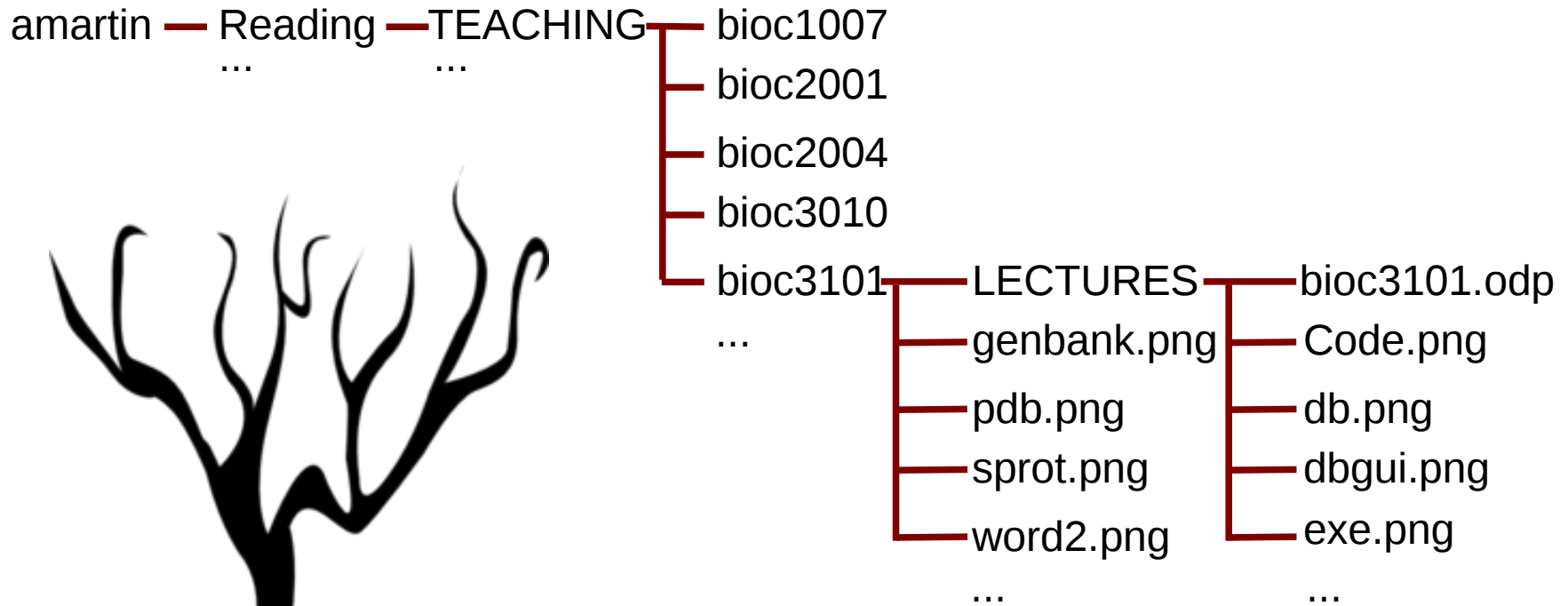
```
    print x[i]
```


Folders, trees and directories

OS GUIs



Trees and directories



Trees and directories

Windows

Each disk (or network share) is the root of the tree:

C:\system

D:\data

Linux/Mac

Everything lives under the same root:

/

/home

/home/amartin

/data

/data/pdb

Using the BASH shell command line

Linux / Mac :- the standard command line
Windows :- git-bash

Navigating the tree

Where am I?

`pwd`

/c/Documents and Settings/amartin

What's in here?

`ls`

Application Data/
Desktop/
...

Cookies/
Favorites/

- `-l` Long format
- `-t` Sort by time
- `-r` Reverse the sort
- `-h` Human format for file sizes

`ls -ltrh`

Navigating the tree

Moving down the tree

```
cd Desktop  
pwd
```

```
/c/Documents and Settings/amartin/Desktop
```

Moving up the tree

```
cd ..
```

Moving across the tree

```
cd ../Start\ Menu  
pwd
```

```
/c/Documents and Settings/amartin/Start Menu
```

Going home

```
cd --or-- cd ~ --or-- cd $HOME  
pwd
```

```
/c/Documents and Settings/amartin/
```

Handling files

View a whole file

```
cat /etc/bash.bashrc
```

View a page at a time

```
less /etc/bash.bashrc
```

Press spacebar for next page
 'b' for previous page
 '>' for last page
 '<' for first page
 '/string' to search for 'string'
 'q' to quit

Copying a file

```
cp /etc/bash.bashrc ~/mybashrc.txt
```


Default input and output

Default input (stdin) is the keyboard

`cat` (no command prompt displayed)

Hello

World

`CTRL-d` (i.e. press and hold CTRL while pressing d)

Default output (stdout) is the screen

`cat ~/mybashrc.txt`

Redirection and pipes

Send the output of a command to a file

```
cat > test.txt          (no command prompt displayed)  
Hello World  
CTRL-d
```

```
cat test.txt
```

```
Hello World
```

Receive input from a file

```
cat < test.txt
```

```
Hello World
```

Sending the output of one program to the input of another

```
cat /etc/bash.bashrc | less
```

Other

Searching: Find lines in a file that contain a string

`grep return /etc/bash.bashrc` (finds all lines containing 'return')

Creating directories

`mkdir newdir`

Removing an empty directory

`rmdir newdir`

Removing a file

`rm myfile`

Removing a directory and all its content

`rm -rf newdir`

Other

Sorting

`sort /etc/bash.bashrc` (alphabetical sort of lines in the file)

Making scripts executable

`chmod +x scriptfile`

Programming in BASH

Renaming a set of files with extension .text to .txt

```
for file in *.text
do
  mv $file `basename $file .text`.txt
done
```