GS-SB-406
Practical Introduction to Programming for Scientists

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Lecture 1:
Introduction

http://blake.bcm.edu/IP18

Course Details (Jan 2018)

- Meets Monday & Friday, 9 - 10:30 AM, N315
- Auditors welcome, but encouraged to register (if permitted)
- Graded
  - 50% Homework & Group Learning, 50% final project
  - Grading will be lenient
- Homework due before each class by email (please email all 3)
  - Michael Bell <James.Bell@bcm.edu>
  - Muyuan Chen <muyuan.Chen@bcm.edu>
  - Steven Ludtke <sludtke@bcm.edu>
- Bring your laptops to class! Some days will be required.
- Group learning typically on Mondays, but may happen on some Fridays
- Class lectures will be video-archived (unless I forget)
- http://blake.bcm.edu/IP18
- There is a special homework for this lecture, to be completed by Sunday night!

TRS-80 Model I

Why should you learn how to program ?

- Something you can’t find in existing software ?
- Make repetitive tasks easier ?
- You want to be a Maker ?

What Can CPUs Do ?

- Store numbers (1 & 0)
  - volatile & nonvolatile storage
- Rearrange stored numbers
- Math
- Simple decisions based on numbers
- Communicate (send and receive numbers to other devices)

8512 computer languages (vs 6909 human)

Machine Language → Assembly Language

Four of the first modern languages (50s):

- FORTRAN (FORmula TRANslator)*
- LISP (LISt Processor)
- ALGOL*
- COBOL (COmmon Business Oriented Language)*

BASIC (1963 - used in 70s-80s)

C (1972)*

C++ (1983)*

Perl (1990)

Python (1991)

Ruby (1992)

HTML (1994)

Java (1995)

* - Compiled languages (usually)

Python ?

PYTHON OOL- developed by Guido van Rossum, and named after Monty Python. (No one Expects the Inquisition) a simple high-level interpreted language. Combines ideas from ABC, C, Modula-3, and ICON. It bridges the gap between C and shell programming, making it suitable for rapid prototyping or as an extension of C. Rossum wanted to correct some of the ABC problems and keep the best features. At the time, he was working on the AMOEBA distributed OS group, and was looking for a scripting language with a syntax like ABC but with the access to the AMOEBA system calls, so he decided to create a language that was extensible; it is OO and supports packages, modules, classes, user-defined exceptions, a good C interface, dynamic loading of C modules and has no arbritrary restrictions.

www.python.org

Why Python ?

- Easy to learn !
- Widely used
- Many available libraries
- Powerful
- Scripting for 3rd party software
- http://www.99-bottles-of-beer.net/

Note: We will use Python 3.x, but Python 2.x is still widely used and available

What to Expect

If you already know some programming

- Learn Python syntax and libraries

If you are starting from scratch

- Read & Modify existing scripts
- Automate tasks
- Write ‘small’ programs from scratch

A Few Apps with Python Scripting

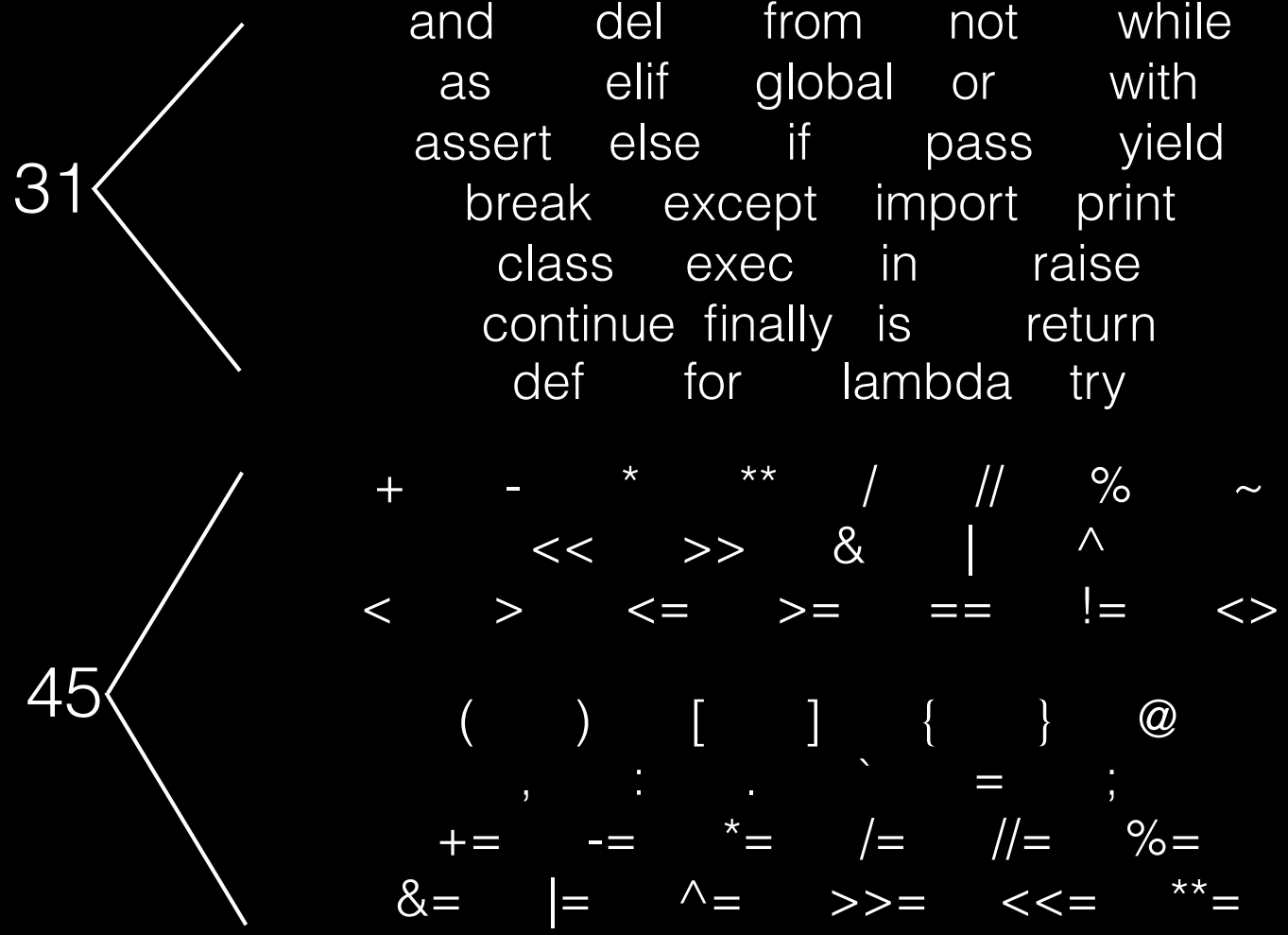
Blender	3-D modeler, animation, post production (free)
Gimp	Photoshop-like graphics editor (free)
Chimera	Structural biology visualization (free)
PyMol	Structural biology visualization (free)
OpenOffice	MS Office clone by Sun (free)
Maya	Professional 3-D Modeling and Animation
Poser	3-D modeling of humans
VTK	Visualization Toolkit (Scientific Visualization, free)
Abaqus	Finite element modeling (free)
EMAN2	Cryo-EM Image Processing (free)
Phenix	X-ray crystallography toolkit (free)
SciPy	Wide range of science/math tools in python (free)
BioPython	Bioinformatics toolkit for Python (free)

Python

- Python is a "high level language"

- **Data storage**
  - ‘simple’ types - numbers, characters
  - compound types - lists, strings, dictionaries, sets, ...
- **Operate on data**
  - statements - a=b*10, print b*5+3, if a>5 : a/=2, ...
  - functions - sin(a), len(x), ...
  - methods (functions on an object) - “abc”.count(“b”)
- **Interact with the outside world**
  - User interactions - raw_input()
  - Disk and other device access - file i/o
  - Networking to other computers

Python Reserved Words



Digital Representation of Numbers

- Bit 0-1
- Byte (char) (8 bits) 0-255
- Word (short) (16 bits) 0-65,535
- Longword (long) (32 bits) 0-4,294,967,296
- Long Longword (64 bits) $0\text{-}1.844 \times 10^{19}$
- Float (32 bits) 10^{38} (7 digits)
- Double (64 bits) 10^{308} (15 digits)

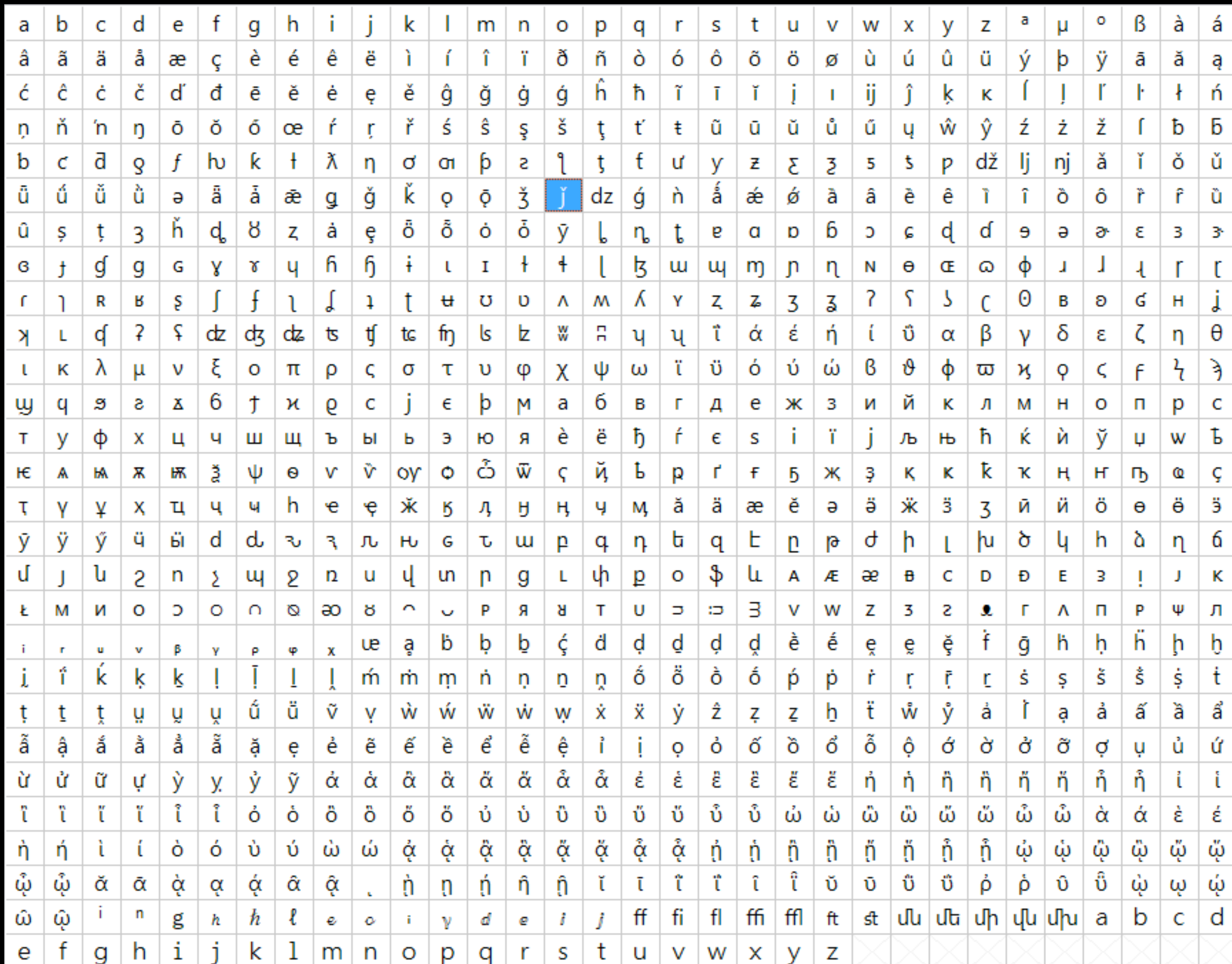
Python Numbers

- integers
  - effectively unlimited
- floating point
  - 64-bit (15 significant figs, $<10^{308}$)
- complex
  - 5.0+3.0j

Characters - ASCII

0	<NUL>	32	<SPC>	64	@	96	`	128	Ä	160	†	192	¿	224	‡
1	<SOH>	33	!	65	A	97	a	129	Å	161	°	193	¡	225	·
2	<STX>	34	"	66	B	98	b	130	Ç	162	¢	194	¬	226	‚
3	<ETX>	35	#	67	C	99	c	131	É	163	£	195	√	227	„
4	<EOT>	36	$	68	D	100	d	132	Ñ	164	§	196	ƒ	228	‰
5	<ENQ>	37	%	69	E	101	e	133	Ö	165	•	197	≈	229	Â
6	<ACK>	38	&	70	F	102	f	134	Ü	166	¶	198	Δ	230	Ê
7	<BEL>	39	'	71	G	103	g	135	á	167	ß	199	«	231	Á
8	<BS>	40	(	72	H	104	h	136	à	168	®	200	»	232	Ë
9	<TAB>	41	)	73	I	105	i	137	â	169	©	201	…	233	È
10	<LF>	42	*	74	J	106	j	138	ä	170	™	202		234	Í
11	<VT>	43	+	75	K	107	k	139	ã	171	´	203	À	235	Î
12	<FF>	44	,	76	L	108	l	140	å	172	¨	204	Ã	236	Ï
13	<CR>	45	-	77	M	109	m	141	ç	173	≠	205	Õ	237	Ì
14	<SO>	46	.	78	N	110	n	142	é	174	Æ	206	Œ	238	Ó
15	<SI>	47	/	79	O	111	o	143	è	175	Ø	207	œ	239	Ô
16	<DLE>	48	0	80	P	112	p	144	ê	176	∞	208	–	240	
17	<DC1>	49	1	81	Q	113	q	145	ë	177	±	209	—	241	Ò
18	<DC2>	50	2	82	R	114	r	146	í	178	≤	210	“	242	Ú
19	<DC3>	51	3	83	S	115	s	147	ì	179	≥	211	”	243	Û
20	<DC4>	52	4	84	T	116	t	148	î	180	¥	212	‘	244	Ù
21	<NAK>	53	5	85	U	117	u	149	ï	181	µ	213	’	245	ı
22	<SYN	54	6	86	V	118	v	150	ñ	182	∂	214	÷	246	ˆ
23	<ETB>	55	7	87	W	119	w	151	ó	183	∑	215	◊	247	˜
24	<CAN>	56	8	88	X	120	x	152	ò	184	∏	216	ÿ	248	¯
25	<EM>	57	9	89	Y	121	y	153	ô	185	π	217	Ÿ	249	˘
26	<SUB>	58	:	90	Z	122	z	154	ö	186	∫	218	/	250	˙
27	<ESC>	59	;	91	[	123	{	155	õ	187	ª	219	€	251	°
28	<FS>	60	<	92	\	124	|	156	ú	188	º	220	‹	252	¸
29	<GS>	61	=	93	]	125	}	157	ù	189	Ω	221	›	253	˝
30	<RS>	62	>	94	^	126	~	158	û	190	æ	222	fi	254	˛
31	<US>	63	?	95	_	127	<DEL>	159	ü	191	ø	223	fl	255	ˇ

Unicode



Characters - Unicode

- All strings in Python3 are Unicode!
- Over 120,000 different characters
- Multiple representations
  - UTF-8, an 8-bit variable-width encoding which maximizes compatibility with ASCII;
  - UTF-16, a 16-bit, variable-width encoding;
  - UTF-32, a 32-bit, fixed-width encoding.

Strings

’string’

”also a string”

””””This too

but this one can span lines””””

”A”+” test”

”A test”

Lists

```
[item1,item2,item3,...]   # items can be anything
a=[0,1,2,3,4,5,6]         # A list of 7 numbers
a[n]                      # nth element in list
a[n:m]                    # sublist elements n to m-1
a[-n]                     # nth item from the end
a[3] -> 3
a[1:4] -> [1,2,3]
a[-2] -> 5
a[2:-2] -> [2,3,4]
a[2]="x" -> [0,1,"x",3,4,5,6]
tuples:  a=(0,1,2,3,4,5,6)     # tuples are immutable
a[3] -> 3
a[3]=5 -> ERROR!
```

List Methods

- append, extend
- del, remove
- count
- index
- reverse, sort

Methods of Strings

- upper, lower, title, capitalize
- count, find, rfind, index
- replace
- split
- regular expressions later...

Sets

- Sets have no order and are unique, but can be iterated over
- set([1,2,3,4,5])
- add, remove, discard, clear
- issubset, issuperset
- union, intersection, difference

Dictionaries

- keys must be immutable, values are arbitrary
- { k1:v1, k2:v2, k3:v3, ... }

  Example:

  a={ 1:2,2:3,”a”:”b”,2.0:3.2,(1,2):”really?” }

  a[1] -> 2

  a[(1,2)] -> “really?”

  a[2] -> 3.2

Dictionary Methods

- has_key
- keys
- values
- items

Some Built-in functions

- int, float, str, list, tuple, set, dict - Converts between types
- range - makes an 'iterator' covering a range
- enumerate
- eval
- raw_input
- len
- max,min
- reversed, sorted
- type, isinstance

Resources

- www.python.org
  - http://docs.python.org/tutorial/
- pypi.python.org
- www.scipy.org

Homework 1
(Auditors too!)

- There is a survey in the homework section at http://blake.bcm.edu/IP17
  Everyone should fill out this form, even if you are informally auditing the class!!!
- Install Anaconda 5 - Python 3.6 (https://www.continuum.io/downloads)
  - Run "jupyter notebook" from the command-line
  - A browser window should open. Select "New [default]"
  - In the new tab/window, you should see: "In [ ]: "
  - Type "import antigravity", then hold down shift and press enter
  - You will know if it worked. If you cannot figure it out, ask for help before Monday! You need to have your laptop at this point before class
- Familiarize yourself with the organization of the documentation at www.python.org (Python 3.x)