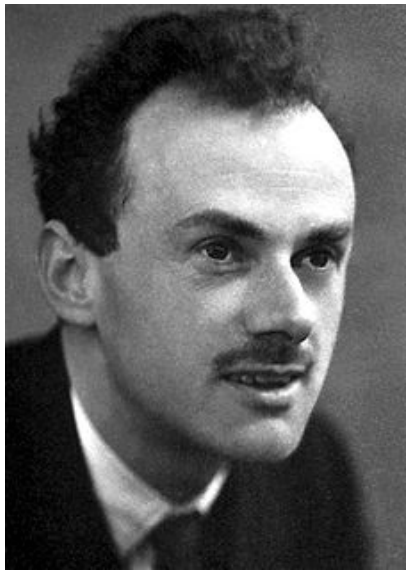
CHEM532 | Jan 12 2014

Modern Techniques in Computational and Theoretical Chemistry

Francesco Evangelista
Emory University

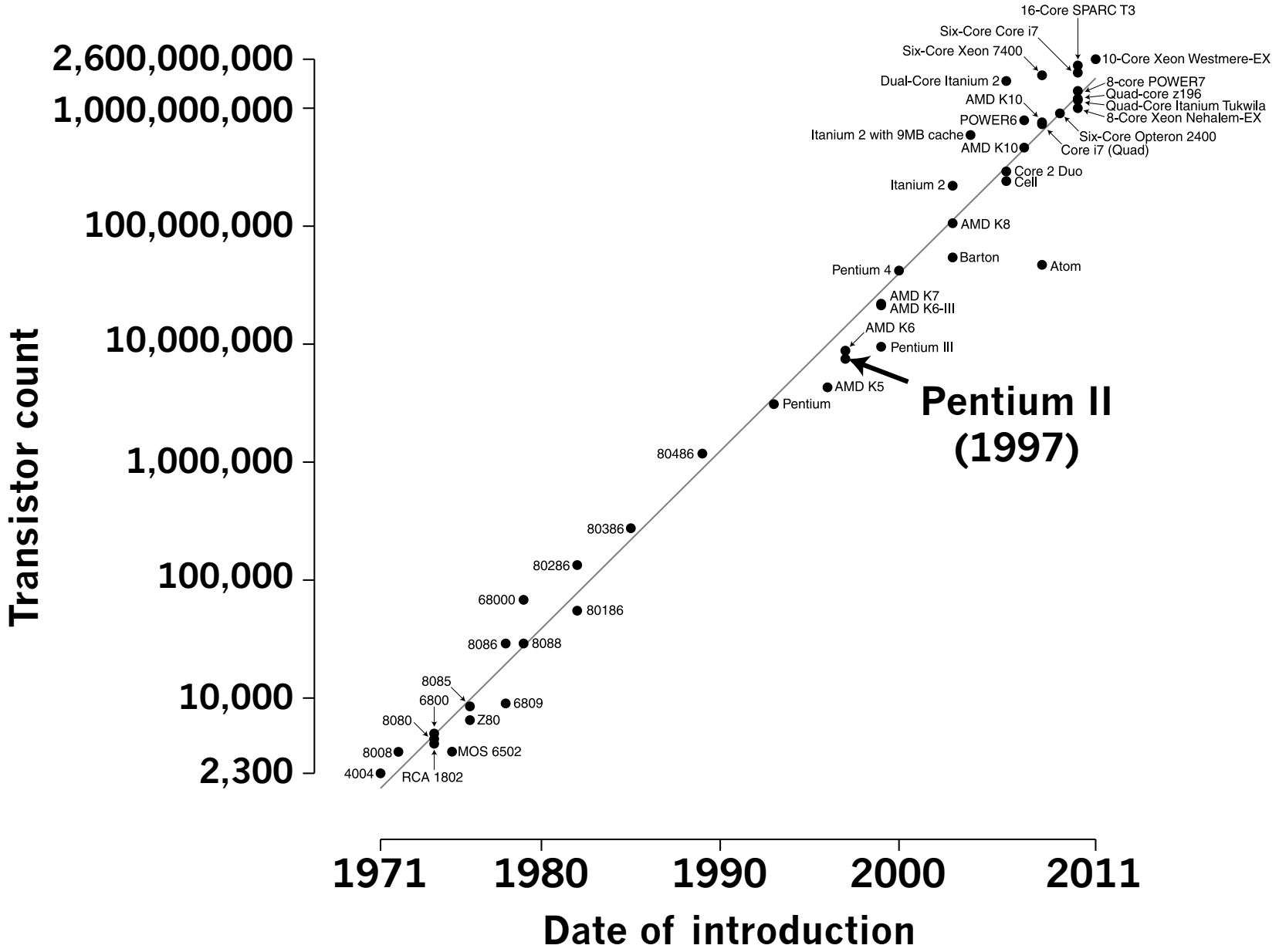
A vision for Computational Chemistry



"The underlying physical laws necessary for the mathematical theory […] of chemistry are thus completely known,*[…]. It therefore becomes desirable that* approximate practical methods *of applying quantum mechanics should be developed […].* "[1]

Dirac, *Proc. R. Soc. Lond. Ser. A* (1929).

Moore's law


Transistor count
2,600,000,000
1,000,000,000
100,000,000
10,000,000
1,000,000
100,000
10,000
2,300
1971
1980
1990
2000
2011
Date of introduction
16-Core SPARC T3
Six-Core Core i7
Six-Core Xeon 7400
10-Core Xeon Westmere-EX
Dual-Core Itanium 2
8-core POWER7
Quad-core z196
AMD K10
Quad-Core Itanium Tukwila
POWER6
8-Core Xeon Nehalem-EX
Itanium 2 with 9MB cache
Six-Core Opteron 2400
AMD K10
Core i7 (Quad)
Core 2 Duo
Cell
Itanium 2
AMD K8
Barton
Atom
Pentium 4
AMD K7
AMD K6-III
AMD K6
Pentium III
AMD K5
Pentium
Pentium II
(1997)
80486
80386
80286
68000
80186
8086
8088
8085
6800
6809
8080
Z80
8008
MOS 6502
4004
RCA 1802

High accuracy

Large molecules

1 cm^{-1} = 0.0029 kcal mol^{-1} = 0.00012 eV

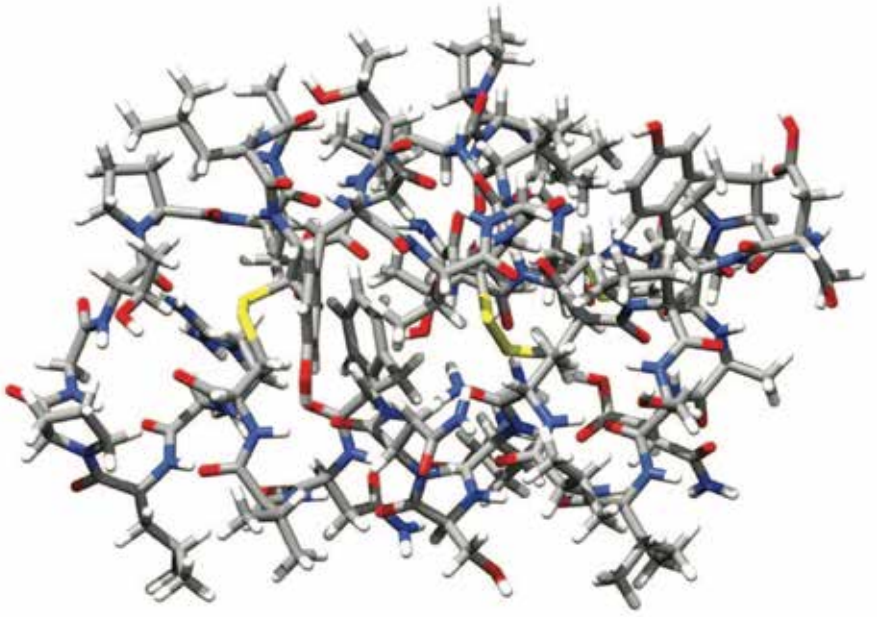
Water, vibrational band origins

MRCI extrapolated to the complete basis set plus core correlation, relativistic effects, Lamb shift, and Born–Oppenheimer corrections
Polyansky *et al. Science* **299**, 539 (2003)

State	Observed (cm^{-1})	Error (cm^{-1})
(010)	1,594.74	−0.32
(020)	3,151.63	−0.56
(030)	4,666.78	−0.78
(040)	6,134.01	−1.06
(050)	7,542.43	−1.41
(101)	7,249.81	0.60
(201)	10,613.35	1.23
All		1.90

Crambin DLPNO-CCSD(T)

644 atoms, 1818 correlated electrons
Riplinger *et al. J. Chem. Phys.* **139**, 134101 (2013)



Course info

- Lectures:
  - Power Point and whiteboard (take notes)
  - Interactive learning (get used to the idea of asking and be asked to answer questions)
  - Quizzes
  - End of class assessment

- Problems sets (which will contain programming projects)

- Programming Projects
  - Learn Python by completing the Python tutorial
    http://www.codecademy.com/tracks/python
  - Harmonic vibrational frequencies
  - Hartree–Fock theory

- Computational project
  - Download a copy of Orca from http://cec.mpg.de/forum/
  - Pick a project related to your research area
  - Geometry optimization, transition states, and vibrational analysis
  - Vibrational energy levels and excited states

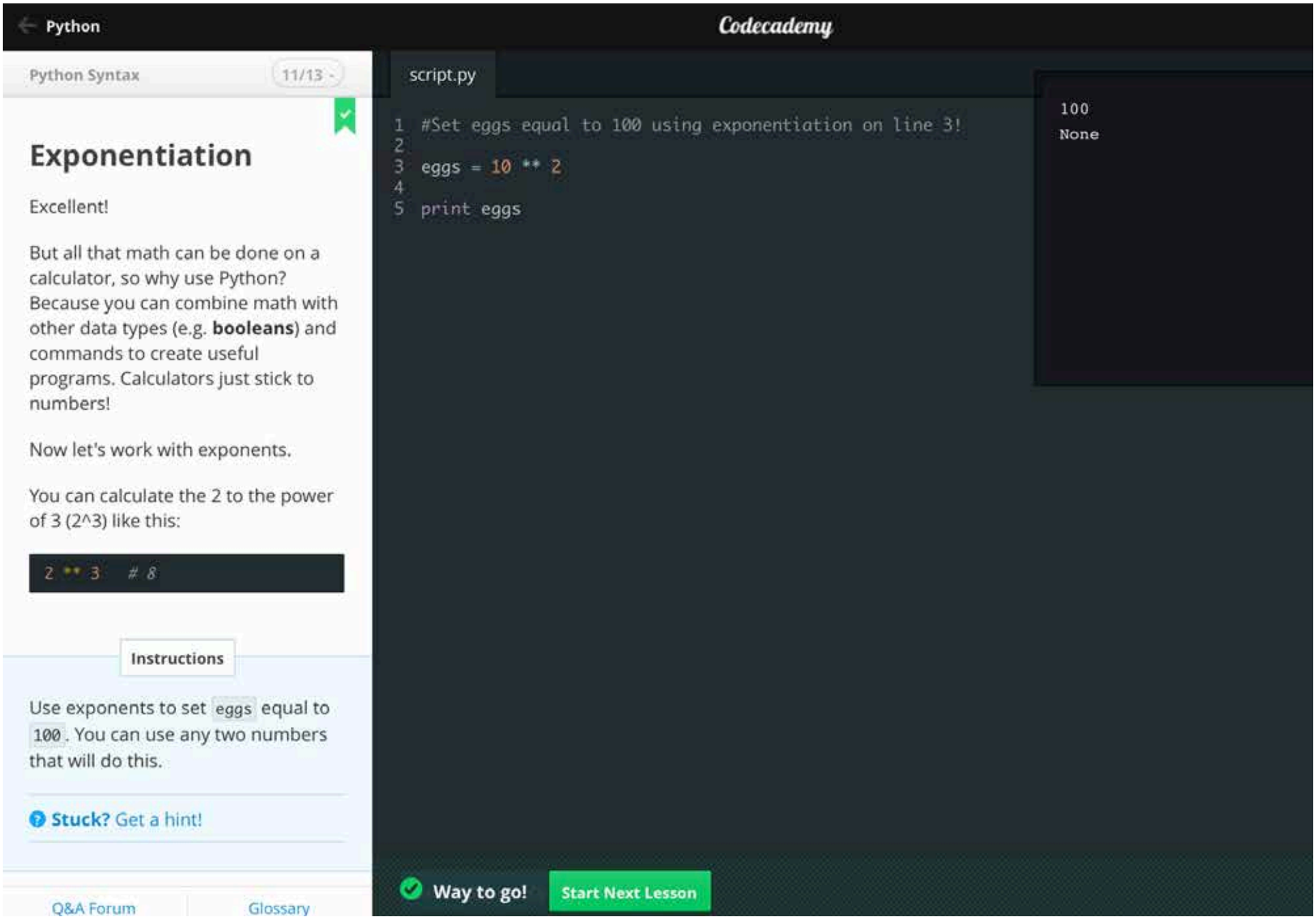
- Get a copy of the syllabus

Python

- Get started today! Download python (www.python.org)

- From a linux, mac terminal
  http://docs.python.org/2/tutorial/interpreter.html
- Windows terminal
  http://docs.python.org/2/faq/windows

- Codecademy Tutorial
- Day 1
  - 1. Python Syntax
  - 2. Tip Calculator
  - 3. Strings & Console Output
- Day 2
  - 5. Conditionals & Control Flow
  - 7. Functions
  - 9. Lists & Dictionaries
- Day 3
  - 12. Lists and Functions
  - 14. Loops
- Day 4
  - 17. Advanced Topics in Python
  - 21. File Input/Output


Python
Codecademy
Python Syntax
11/13
Exponentiation
Excellent!
But all that math can be done on a calculator, so why use Python? Because you can combine math with other data types (e.g. booleans) and commands to create useful programs. Calculators just stick to numbers!
Now let's work with exponents.
You can calculate the 2 to the power of 3 (2^3) like this:
2 ** 3 # 8
Instructions
Use exponents to set eggs equal to 100. You can use any two numbers that will do this.
Stuck? Get a hint!
Q&A Forum
Glossary
script.py
1 #Set eggs equal to 100 using exponentiation on line 3!
2
3 eggs = 10 ** 2
4
5 print eggs
100
None
Way to go!
Start Next Lesson