Experience with Using Python as a Primary Language for Teaching Scientific Computing at the University of Oslo

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Abstract

This essay explains why and how we have chosen Python as the language of choice for teaching scientific computing at the University of Oslo. By teaching students Python from day one, various bachelor programs have taken advantage of this knowledge and reformed classical science courses by using programming and numerical simulation to solve mathematical problems. We have learned several lessons:

- The choice of Python as a teaching language for scientific computing has been a great success and is highly recommended.

- It is possible to treat quite advanced problems very early in the studies, e.g., implement an object-oriented toolbox for solving a large class of nonlinear vibration problems.

- Replacing classical mathematical solution techniques by programming and numerical simulation in science courses is indeed challenging, but possible and natural. The experience is very positive and such reforms are strongly encouraged.

- Students come with all sorts of laptops. Force everyone to use Ubuntu as this minimizes the technical hazzle with installing complicated mathematical software.

We started with a course on Python scripting

In 1999, I started a course (IN228, renamed to INF3331) about scientific scripting at the University of Oslo. The purpose was to use a real scripting language, primarily Perl, to automate execution and archival of large-scale simulation studies. Besides dramatically reducing tedious manual work and ensuring consistent association of results with input data, such automation is also key to reproducible science since the script that performs the experiments documents everything that is needed to reproduce the results. The course also covered many typical "administrative tasks" that a computational scientist must deal with, such as interpreting file formats and making user interfaces of various kind.

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Within a couple of years, we naturally moved from Perl to Python as the primary scripting language, simply because Python did the same as Perl just with a more readable syntax that made the programs easier to go back after six months. Students picked up Python significantly faster than Perl, and we realized the pedagogical strengths of the Python language. I wrote a book for the course, but the publisher was initially only modestly interested because Python was still an insignificant language. Our gut feeling, however, said that Python with time would gain a significant position in the science and engineering community. At the time of this writing, this is a fact and the mentioned book turned out to be a best-seller in its category. More than 1500 students have been educated in Python through this course and are now active in industry.

The course addressed experienced Fortran, C, C++, or Java programmers and aimed at teaching them the power of a dynamically typed environment. Early in the 2000s, our research group started using Python for scientific computations, not only scripting. Our students used Python (with NumPy, SciPy, and friends) as a MATLAB replacement and migrated slow parts of the code to Fortran or C++ when needed. It stroke us that students should learn about this effective numerical computing environment as early as possible.

We chose Python for learning computer programming

Most universities ask the computer science department to provide an introductory programming course, and very often the offer is a standard Java course. Sometimes the choice is C, C++, or perhaps something more exotic like Scheme. Beyond the very basics of programming, the content is usually typical computer science algorithms rather than numerical algorithms. The result is often that students for all practical purposes must relearn to program when they meet programming in science courses, and then the language is usually MATLAB, Fortran, C, or C++.

At the University of Oslo, the introductory Java course was not well synchronized with the needs in science courses and the mentioned relearning of programming consumed much time when they met a totally different language and totally different applications of programming at the end of the bachelor studies. We therefore decided around 2006 to develop an introductory programming course that could lay a firm foundation for continued programming in all later courses where the teaching would benefit from integrating numerical simulations. A part of the idea was to teach programming in the context of relevant algorithms like numerical integration, differentiation, solution of differential equations, and Monte Carlo simulation.

The introductory programming course was scheduled for the very first semester, meaning that the students would learn to program and use the computer to solve mathematical problems from day one. But what should be the language of choice? MATLAB or C++ were obvious candidates because of their popularity. These two languages are, however, very different in nature, and it is not natural to integrate them in a course. Python, on the other hand, can be

used for MATLAB-style programming and object-oriented or generative C++-style programming. In this way Python provides a natural glue between different programming styles. We also knew that Python was much easier to use and teach than C++. The most convincing argument was, nevertheless, that Python may act as a MATLAB replacement for students and professors, doing the same things as MATLAB, and for free, but with a much more powerful programming language at disposal.

Again I wrote a book for the introductory programming course, this time addressing newcomers to programming and concentrating the examples on numerical computing. Needless to say, there were many skeptics: Python was of marginal interest to scientific computing, Python was a bad first language, mixing programming and mathematics is inferior to first mastering calculus and Java separately, etc. etc.

The course is now a huge success. Since 2007, more than 1000 students have passed the exam and used the programming technology to solve mathematical problems in about 20 other courses in the Bachelor programs at the University of Oslo. The introduction of programming and numerical simulation in all these other courses was a huge undertaking known as the Computing in Science Education project. This project has attracted worldwide attention as it represents a long-awaited reform of the science education. The idea is trivial: let programming and computer simulations change the curriculum! However, the implementation among professors is extremely demanding most places. The fortunate situation in Oslo is that professors across disciplines have managed to collaborate on how programming and simulation can be integrated in classical courses and used to replace the classical strong attention on complicated and specialized mathematical techniques for very simplified physical problems. Recently, the Computing in Science Education project has been acknowledged by the University and the government in Norway through prestigious awards and generous funding. The ideas are being implemented at other Norwegian colleges and universities as well as at several institutions abroad.

Impact of Teaching Python

The world is changed only when people do new things. When students learn Python, they bring this knowledge to later courses and then to industry. Their knowledge automatically creates a demand for using the tools they prefer. Many companies in the Oslo region that apply Python today discovered the language through new employees who had picked up Python in the scripting course. Similarly, students create Python examples and projects in other courses and thereby attract attention to the tool and its applications.

The science education at the University of Oslo puts much emphasis on learning other languages, in particular MATLAB, R, C, C++, and Fortran. We teach (a subset of) Python in a way that eases the transition to and from MATLAB. For high performance we emphasize reusing Fortran and C libraries from Python or migrating slow Python code to compiled languages. Our experience

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shows that users who gain a good knowledge of Python tend to prefer that language and do as much as possible in Python before the quest for high performance demands migration of (usually small) parts of the code to a compiled language. It seems that many students and professors, when their knowledge of Python is at the level of their MATLAB skills, steadily drift to do most of their work in Python. This is a sign of a kind of gravity force, which we believe is rooted in Python's syntax, powerful expressiveness, and rich set of libraries.

The described trend among students and professors are also found in industry: Python steadily eats of the MATLAB market because people find the language stronger and more convenient. Our efforts in teaching and professional use of Python contribute to the observed exponential growth. MATLAB has in my opinion been the single most important invention in scientific computing, and Python represents a kind of "free MATLAB" with a more powerful programming language.

We let the students play with advanced problems

As mentioned, we start day one when the 19-year old new students arrive at the University. About 300 students enter courses on classical calculus, numerical calculus, and programming of the latter. The programming course covers basic MATLAB-style procedural programming in the first half of the fall semester, while the second half is spent on class programming (classes and object-oriented programming were invented in Oslo so we have no other choice!), statistical simulations, and ordinary differential equations. The final project is to create a flexible, object-oriented toolbox for studying nonlinear vibration problems described by the standard model

$$m\ddot{x} + f(\dot{x}) + s(x) = F(t)$$

Many reviews of the course book claim that the book is quite advanced and may fit the graduate level. However, most of the book is in fact covered the very first semester in Oslo. This works well and the course has received excellent student critiques. Scientists usually think of Monte Carlo simulation and nonlinear differential equations as advanced topics, not belonging to first semester courses, but the methods and their applications can be exposed in very intuitive ways suitable for newbies. At least the students can train their programming skills on such problems and be able to produce solutions to what many traditionally think of as advanced problems. However, a deeper understanding of what they actually do needs to wait until they master a broader set of courses.

We use Ubuntu to minimize installation problems

Many fear to introduce programming and simulation in courses because there are so many technical details. For example, how shall students install Python and 30 software packages on their personal laptops? Elaborating a bit on this problem setting quickly scares any teacher. We have found a solution that

has proven to be successful over the last four years: *force all students to use Ubuntu* and provide support for Ubuntu only!

Mac users typically run Ubuntu in a virtual machine (VirtualBox, or preferably, VMWare Player or VMWare Fusion), while Windows users can run a virtual machine or have a dual boot. The Wubi software makes installing the dual boot solution very easy. On Ubuntu we have one package (`python-scitools`) that installs everything the students need in one command. Later courses can just provide a one-line command with their needs for additional packages.

There are several reasons why we dare to force the use of Ubuntu:

1. Ubuntu (or more precisely, Debian Linux) has the largest collection of mathematical software today.

2. Mathematical software is often complex to install, but on Ubuntu this is done by a one-line command.

3. Ubuntu is easier for students to operate than other Linux/Unix systems (especially Mac OS X).

4. Ubuntu's graphical interface is very similar to Windows or Mac OS X.

5. Ubuntu (or more precisely, Unix/Linux) provides more powerful support for programming in general than Windows or Mac (in my opinion).

Soon we expect supercomputing in the cloud to be a reality. Then one can just upload the Ubuntu image (running in a virtual machine) to the cloud service and avoid tedious installation processes. By archiving the image along with scientific results, one can at any time in the future rerun simulations - the complete operating system, all the needed software, and all data reside in the image.

So far, I have not heard one single negative comment that we support Ubuntu only. When we tried to support Unix, Linux, Windows, and Mac, there were a lot of complaints from students that they did not have access to the right software and that technical problems with computers stole too much attention. These complaints have simply disappeared with the standardization on Ubuntu. This is very surprising to me (and most others), but a fact.

Resources

- "PDF version" of this eassy: "http://hplgit.github.com/teamods/uiopy/uiopy.pdf"

- The book Python Scripting for Computational Science

- The book A Primer on Scientific Computing with Python

- Student information on our introductory programming course where Python is used

- The Computing in Science Education reform of science courses

- How to install Ubuntu on any computer using VMWare Fusion

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