Performance of Python runtimes on a non-numeric scientific code

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Abstract—The Python library FatGHoL [FatGHoL] used in [Murri2012] to reckon the rational homology of the moduli space of Riemann surfaces is an example of a non-numeric scientific code: most of the processing it does is generating graphs (represented by complex Python objects) and computing their isomorphisms (a triple of Python lists; again a nested data structure). These operations are repeated many times over: for example, the spaces $M_{0,k}$ and $M_{1,k}$ are triangulated by 4'583'322 and 747'664 graphs, respectively.

This is an opportunity for every Python runtime to prove its strength in optimization. The purpose of this experiment was to assess the maturity of alternative Python runtimes, in terms of: compatibility with the language as implemented in CPython 2.7, and performance speedup.

This paper compares the results and experiences from running FatGHoL with different Python runtimes: CPython 2.7.5, PyPy 2.1, Cython 0.19, Numba 0.11, Nuitka 0.4.4 and Falcon.

Index Terms—python runtime, non-numeric, homology, fatgraphs

1 INTRODUCTION

The moduli space $M_{g,n}$ of smooth Riemann surfaces is a topological space which has been subject of much research both in algebraic geometry and in string theory. It is known since the ’90s that this space has a triangulation indexed by a special kind of graphs [Penner1988], [Kontsevich1992], [ConantVogtmann2003], nicknamed “fat graphs”.

Since graphs are combinatorial and discrete objects, a computational approach to the problem of computing topological invariants of $M_{g,n}$ is now feasible; algorithms to enumerate fatgraphs and compute their graph homology have been devised in [Murri2012] and implemented in Python.

We propose an experiment whose purpose is to assess the maturity of alternative Python runtimes, in terms of:

(a) compatibility with the language as implemented in CPython 2.7, and
(b) performance speedup.

In particular, we were interested in the possible speedups of a large non-numeric code.

2 EXPERIMENT SETUP

The FatGHoL <http://fatghol.googlecode.com/> [FatGHoL] program was used as a test code. FatGHoL computes homology of the moduli spaces of Riemann surfaces $M_{g,n}$ via Penner-Kontsevich’s fatgraph simplicial complex [Penner1988], [Kontsevich1992]. Homology is one of the most important invariants of topological spaces. There are several homology theories but they all share this computational procedure outline: given a vector space of (generalized) simplex chains and a boundary operator, which is by definition a linear operator $D$ such that $D^2 = 0$, the homology space is by definition $\ker D / \text{Im} D$. In graph homology, however, it is the computation of these simplices and boundary that takes up the largest fraction of compute time: the simplex chains are defined as formal linear combinations of graphs, and the boundary operator maps a graph into a linear combination of graphs obtained by contracting its edges. Thus, explicit construction of the simplices requires enumerating all distinct isomorphism classes of fatgraphs, and then computing their mutual relationships upon contraction of edges.

The FatGHoL program runs in three stages:

1. generate fatgraphs,
2. explicitly compute the boundary operator in matrix form,
3. actually solve the homology linear system.

The last step has been disabled in the test code as it is implemented in C++ for speed. What remains is 100% pure Python code that runs on Python 2.6+ (but could run on 2.5 with minimal modifications).

FatGHoL involves a large number of graph isomorphism computations: especially during fatgraph generation, each candidate fatgraph needs to be compared to all fatgraphs already discovered, in order to avoid duplicates. In later stages, the isomorphism computations are cached in memory, but in step 2 additional data is created for each graph, in order to pass from fatgraphs to simplices.

It is worth noting that the FatGHoL code exercises many of Python’s advanced data manipulation features, like list and dictionary comprehensions, slicing, etc. but does not use any kind of tight nested loops of the kind normally featured in numeric codes.

Profiling data show more precisely how much work is done at the Python level in the simplest case $M_{0,4}$. The following listing shows profiling data extracted from a complete...
run of FatGHoL on CPython 2.7.5: 15787953 function calls (15728052 primitive calls) were effected in 39.572 seconds; the top 10 most called functions, ordered by call count are:

```
ncalls  tottime  filename:lineno(function)
2216088  2.175  rg.py:227(<genexpr>)
968575  0.819  rg.py:143(ls_loops)
775362  0.839  cyclicseq.py:88(__getitem__)  
775362  0.634  rg.py:170(other_end)
722308  3.438  combinatorics.py:368(___init__)  
539039  1.689  cyclicseq.py:112(__getslice__)  
506075/447917  0.745  cache.py:181(wrapper)
476134  1.122  combinatorics.py:441(rearranged)
385725  0.355  rg.py:137(__init__)  
345740  0.849  rg.py:168(__first_unused_corner)
```

The FatGHoL code was run with seven different alternative Python runtimes:

- CPython 2.7.5;
- Cython 0.19.1;
- Cython 0.19.1 in "pure Python mode";
- Falcon 0.05;
- Nuitka 0.4.4;
- PyPy 2.1;
- Numba 0.10.0 and 0.11.0 with @autojit.

A detailed description of each of these is given in a later section; Table 1 provides an overview of the installation and usage features of the different runtimes. The code used to install the software and run the experiments is available on GitHub at https://github.com/riccardomurri/python-runtimes-shootout.

Except for Cython in "pure Python mode" and Numba, all runtimes run the unmodified Python code of FatGHoL. Cython in "pure Python mode" requires the addition of decorators to the Python code that specify the types of function arguments and local variables to increase speedup of selected portions of the code. Similarly, Numba uses the decorators @jit or @autojit to mark functions that should be compiled to native code (the difference between the two decorators is that @autojit infers types at runtime, whereas @jit requires the programmer to specify them\(^1\)); we only used the @autojit decorator to mark the same functions that were marked as optimization candidates in the Cython experiment.

Each Python runtime was run on 4 test cases: computing the homology of the \(M_0,5, M_1,3, M_2,1\) moduli spaces. The test cases take from 0.20s to more than 2 minutes of runtime with CPython 2.7. Each test case was run 10 times and the best time and lowest RAM occupation are reported in the summary tables below.

### 3 Results

Falcon and Numba could not run the code (see details in a later section) and thus do not appear in the report below.

For each runtime, the total used CPU time and memory were measured: results and summary graphs are given in figures 1 and 2. Detailed comparisons are given in the other figures.

The CPU time data prompt a few observations:

- PyPy gives the best results, provided the code runs long enough to discount for the startup time of the JIT compiler. Given enough time, the JIT compiler gives extremely good results, with speedups of 100% to 400% relative to CPython in the \(M_0,5\) and \(M_1,3\) cases. In other words, for the JIT approach to pay off, the code needs to perform many iterations of the same code path (this is certainly the case for FatGHoL), because compiling a single function to native code takes a non-negligible amount of time. The break-even point for the FatGHoL code seems to be around 5 seconds of runtime: on \(M_2,1\), the CPU time taken by CPython and PyPy are almost equal.
- Cython gives consistently about a 30% speedup on unmodified Python code. However, the "pure Python mode", in which Cython takes variable typing hints embedded in the code does not seem to give any advantage: results of the two runs are not significantly different. This might be related to a bug in the current version of Cython, see details in a later section.

The large memory consumption from PyPy and Nuitka stands out in the memory data of figure 2. On the other hand, there is no significant increase in memory usage between CPython and Cython.

The large memory usage of PyPy can be explained by the fact that the JIT infrastructure must keep in memory the profile and traces for all the code paths taken. In any long-running program, the memory should eventually reach a steady state and not increase any further; it should be noted however, that in these benchmarks the memory used by the PyPy JIT framework dwarfs the memory used by the program itself.

We have no explanation for the large memory consumption of Nuitka.

### 4 Runtime Systems Details

#### 4.1 Cython 0.19.1 <http://cython.org/>)

Cython is a compiler for a superset of the Python language. It translates Python modules to a C or C++ source that is then compiled to a native code library that CPython can load and use. Cython optimizes best when users decorate the source code with hints at the types of variables and functions; it can also translate unmodified Python code, but then no type inference is performed. Cython allows a variety of ways for giving these type hints; its so-called "pure Python" mode requires users to insert functions and variable decorators in the code: the Cython compiler can act on these directives, but the CPython interpreter will instead load a cython module which turns them into no-ops.

We tested Cython twice: on the unmodified Python sources, and with hinting in the "pure Python" mode. The graphs show however very little difference between the two modes; this could be a consequence of Cython defect ticket #477.

Cython does its best when the source code is annotated with its extended keywords, which allow specifying the types of variables (which allows optimizations, e.g., in loops), or marking certain functions as C-only (which saves time when dereferencing variables). This extended markup can be provided either in the sources, or in additional .pxd files. We have not done this exercise, however, as the amount of coding

\(^1\) Note that in more recent versions of Numba, the two decorators have been fused into one: @jit uses the supplied types, or infers them if none are given.
time required to properly mark all functions and variables is quite substantial.

4.2 Falcon 0.05 [https://github.com/rjpower/falcon]
Falcon is a Python extension module that hacks into a CPython interpreter and changes the execution loop, implementing several optimizations (for instance, using a register-based VM instead of a stack-based one) that the Falcon authors think should be used in the upstream CPython interpreter too. However, Falcon is still in early stages of development and crashes on FatGHoL code with a segmentation fault.

4.3 Numba [http://numba.pydata.org/]
As its website states:

Numba is an optimizing compiler for Python; it uses the LLVM compiler infrastructure to compile Python syntax to machine code. It is NumPy-aware and can speed up code using NumPy arrays. Other, less well-typed code will be translated to Python C-API calls effectively removing the “interpreter” but not removing the dynamic indirection. Numba is also not a Just-In-Time compiler.

Numba requires the code developer to use either the @autojit (use run-time type info) or the @jit (explicitly provide type information) decorators to mark those functions that should be compiled. For our experiment, we used the decorator @autojit on all functions that were decorated also in the Cython test.

Versions 0.10.0 and 0.11.0 of Numba were tested; we could not get either version to work.

Numba version 0.10.0 dies with an internal error (“TypeError: type_container() takes exactly 1 argument (3 given)”, reported as Issue #295 on Numba’s GitHub issue tracker), that has been fixed in version 0.11.

However, Numba 0.11.0 with a "NotImplementedError: Unable to cast from [ i64, i8* ]* to [ i64, i8* ]" message. This has been reported as Issue #350 on the issue tracker and is waiting for a fix.

4.4 Nuitka 0.4.4 [http://www.nuitka.net/]
Nuitka translates Python (2.6+) into a C++ program that then uses libpython to execute in the same way as CPython does, in a very compatible way. Although still in development, Nuitka claims that it already:

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TABLE 1: Comparison of installation features of the Python runtimes. \(^a\) Plus 123MB for the CPython interpreter, which is anyway needed. \(^b\) Does not need the CPython interpreter in addition, as all others do.

| Runtime   | Cython 0.19.1 | Falcon 0.05 | Nuitka 0.4.4 | Numba 0.11.0 | PyPy 2.1 |
|-----------|--------------|-------------|--------------|--------------|-----------|
| Installed size (MB) | 30 \(^a\) | 14 \(^a\) | 25 \(^a\) | 97 \(^a\) (+ 518MB of LLVM 3.2) | 162 \(^b\) |
| Install script length (SLOC) | 6 | 8 | 10 | 24 | 19 |
| Usage documentation | extensive | minimal | short how-to to explain the different compilation options available | minimal, mostly examples | none |
| Porting/optimization documentation | extensive | none | list of optimizations that the runtime does (or will) support | none | provides only a list of compatibility issues; I could find no list of Do’s and Don’t-s for better speed in PyPy |

Table 1: Comparison of installation features of the Python runtimes. \(^a\) Plus 123MB for the CPython interpreter, which is anyway needed. \(^b\) Does not need the CPython interpreter in addition, as all others do.
Comparison of the total CPU time used by each runtime on the different test cases. The x-axis shows values in seconds. Note that the y-axis is drawn on a logarithmic scale!

Comparison of the total RAM used by each runtime on the different test cases. The x-axis is sorted so that the RAM usage for CPython 2.7.5 is ascending. The y-axis shows values in MBs (smaller is better).

Comparison of the total CPU time used by each runtime on the M0,4 test case. The x-axis shows values in seconds.

Comparison of the total CPU time used by each runtime on the M0,5 test case. The x-axis shows values in seconds.

Comparison of the total CPU time used by each runtime on the M1,3 test case. The x-axis shows values in seconds.

Comparison of the total CPU time used by each runtime on the M2,1 test case. The x-axis shows values in seconds.

Comparison of the total RAM usage by each runtime on the M0,4 test case. The x-axis shows values in MBs.

Comparison of the total RAM usage by each runtime on the M0,5 test case. The x-axis shows values in MBs.

Comparison of the total RAM usage by each runtime on the M1,3 test case. The x-axis shows values in MBs.
create[s] the most efficient native code from this. This means to be fast with the basic Python object handling.

Results of this experiment do not seem to corroborate this claim.

4.5 PyPy 2.1 <http://pypy.org/>

PyPy is a Python language interpreter with a Just-In-Time compiler (and many other features!). It can thus translate repetitive Python code into native code on the fly. PyPy must first be bootstrapped by compiling itself, which takes a lot of time and RAM, but then it is a drop-in replacement for the python command and just works.

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