1 Background

In many applications a function has to be called very often inside a loop. One such application in numerical analysis is the finite element method (FEM) for the approximate solution of a partial differential equation (PDE). For example we would like to approximate the solution \( u : \Omega \rightarrow \mathbb{R} \) of the PDE

\[
- \nabla \cdot (a \nabla u) + b \cdot \nabla u + cu = f \quad \text{in } \Omega \\
u = g \quad \text{on } \partial \Omega
\]

where \( \Omega \subseteq \mathbb{R}^d \) is a \( d \)-dimensional domain with boundary \( \partial \Omega \) and \( a, c, f : \Omega \rightarrow \mathbb{R}, b : \Omega \rightarrow \mathbb{R}^d \) and \( g : \partial \Omega \rightarrow \mathbb{R} \) are given functions with special properties that will not be discussed here. In FEM a domain is discretized into a mesh by splitting the domain into "simple" geometric shapes (intervals, triangles, tetrahedrons, ...). Along with special functions (usually piecewise polynomials) these shapes are called elements. A system of linear algebraic equations \( Ax = b \) is obtained by computing integrals on each element and sorting them into a large (and usually sparse) "system" matrix \( A \) and right hand side (RHS) \( b \).

From a computational point of view this can be achieved by writing a function \texttt{getElementIntegrals(...)\texttt{}} that computes all necessary integrals on one element and is then called within a loop for each element of the mesh. A corresponding Python code could look like this:

```python
for el in mesh:
    elMat, elRHS = getElementIntegrals(el,a,b,c,f,g)
    # process entries of elMat and elRHS by sorting them
    # into a "big" matrix and right hand side.
```

*\texttt{gaul@math.tu-berlin.de, http://www.math.tu-berlin.de/78347. This work is licensed under the creative commons license CC-BY-3.0. All used source code files are published under GPL 3.0 in the git repository https://bitbucket.org/andrenarchy/funcall.} \texttt{\textcopyright 2012 arXiv:1202.2736v1 [cs.PL] 13 Feb 2012}
Now imagine that the mesh is very fine, i.e. the number of elements in the mesh is large. For example a uniform tetrahedral discretization of the unit cube \([0,1]^3\) with grid size \(h = 1/n\) \((n \in \mathbb{N})\) results in a mesh consisting of \(6n^3\) tetrahedral elements. The function \(\text{getElementIntegrals}\) is thus called \(6n^3\) times.

Especially in interpreted programming languages like MATLAB, Octave or Python a function call may be very time-consuming. By \textit{function call} we mean the setup needed for the function to start executing the actual function code in the function’s body and cleaning it up afterwards. This includes possible copying of memory and dynamic type checking for the parameters passed to and returned from the function.

In the above setting the functions \(a, b, c, f, g\) and even \(\text{getElementIntegrals}\) can often be evaluated in a fast way. However, the function call itself may exhibit an overhead that consumes far more time than the actual function code. In this report we present results of function call benchmarks for programming languages or interpreters often used in numerical analysis: MATLAB/Octave, Python and C. While C is a compiled language and optimizations are possible even on a very low level, MATLAB and the free software alternative Octave are interpreted languages and mainly draw on automated optimization and low-level improvements are usually only possible by switching to plain C, C++ or Fortran with so-called mex-files. In contrast, in the interpreted language Python time-critical parts can be compiled with Cython – the C-Extensions for Python \([1]\). Cython’s syntax is very similar to Python’s and introduces static typing as well as the ability to call C code easily.

Here we present a benchmark that helps to identify and quantify optimization potentials with respect to time consumption caused by function calls in the mentioned languages. Section 2 describes the setup of the benchmark and Section 3 presents and discusses the results.

## 2 Benchmark setup

The situation outlined in Section 1 can be boiled down to a function that is called in a loop very often. For benchmarking the overhead of the function call itself it is reasonable to make the function body as simple as possible. Therefore, we will use a function that accepts one double precision floating-point number and returns its square. We ran separate tests for several types of function definitions that are available in the used programming languages. The different options are enumerated for later reference.

### MATLAB and Octave

Option 1. (a) The called function defined in an external .m-file:

```matlab
function result = fun_external(a)
    result = a*a;
end
```

The loop is defined in a separate file:

```matlab
function result = loop_external(n)
```

2
result = zeros(n,1);
for i=1:n
    result(i) = fun_external(i);
end
end

(b) Both functions from (a) are placed in the same file consecutively.
(c) A nested function definition in the body of the calling function is used, that is the called function is placed *inside* the body of the loop function:

```
function result = loop_nested(n)
    result = zeros(n,1);
    for i=1:n
        result(i) = fun_nested(i);
    end

    function ret = fun_nested(a)
        ret = a*a;
    end
end
```

(d) Anonymous function definition in the body of the calling function:
```
fun_anonymous = @(a) (a*a);
```

**Python**

Python is an interpreted language but can be tuned by writing time-critical parts in Cython [1]. With Cython one can blend Python code and C code easily. We take a closer look at the following options for implementing the loop and the called function:

Option 1. The called function can be implemented

(a) together with the loop function in the same .py-file or

(b) in a separate .py-file and imported in the .py-file implementing the loop.

Option 2. The loop can be implemented with a numpy array [3] in

(a) plain Python:
```
def loop(n):
    result = numpy.empty(n)
    for i in xrange(0,n):
        result[i] = fun_samefile(i+1)
    return result
```

or in

(b) Cython where the code still is plain Python code as in (a) or in
(c) Cython enriched with static typing:

```python
def loop(n):
    cdef numpy.ndarray[numpy.double_t] result = \
        numpy.empty(n)
    cdef int i
    for i in xrange(0,n):
        result[i] = fun_samefile(i+1)
    return result
```

Note that the `result` array and the `i` variable are now typed which allows Cython to address the elements of the numpy array in the loop efficiently.

Option 3. Similarly, the called function can be implemented in

(a) plain Python:

```python
def fun(a):
    return a**2
```

or in

(b) Cython where the code still is plain Python code as in (a) or in

(c) Cython enriched with static typing:

```python
cpdef double fun(double a):
    return a**2
```

If the function is imported in the .py-file running the loop then an additional .pxd-file with the corresponding function declaration should be provided. A .pxd-files works like a C header file and in our case simply contains the line

```python
cpdef double fun(double a)
```

Several combinations are not possible and are thus omitted. For example, option 1 (a) with option 2 (a) and option 3 (b) are impossible because both the loop and the called function are compiled with Cython if they are defined in the same file).

C

Option 1. (a) The function is defined in the same .c-file as the loop and compiled with the options `-O3 -fomit-frame-pointer`. The function code is

```c
double fun(double a) {
    return a*a;
}
```

while the loop code is
double* loop (int n) {
    double* result = (double*) malloc (sizeof(double)*n);
    for (int i =0; i<n; i++)
        result[i] = fun(i);
    free(result);
    return result;
}

(b) The function is compiled in a shared library (.so-file) which is then dynamically linked to the compiled loop function. The compiler options are the same as for (a).

For further details we refer to the source code [2].

3 Benchmark results

In this section we present results of the benchmark setup described in Section 2 conducted with the languages/interpreters

- MATLAB 2011b
- Octave 3.2.4
- Python 2.7.2
- Cython 0.14.1 (C-Extensions for Python)
- C with GCC 4.6.1.

All experiments have been carried out on a Intel Core i5 M540 CPU running at 2.53 GHz with Ubuntu 11.10. We computed $a^2$ for $a = 1, \ldots, 10^7$ with all possible variations of implementations with the options presented in 2. By using this test setup we wish to identify and quantify possibilities for optimization with respect to time consumption caused by function calls. The experiment was repeated 10 times and the arithmetic mean of the measured timings are presented in Table 1.

The files used for the experiments are published [2] under GPL3 so further results can be produced with later versions of the above software and on different hardware.

Unsurprisingly, both C implementations with enabled compiler optimizations are the fastest implementations in this benchmark. The fact that Octave is slower with function calls than MATLAB is also well-known. More interesting is the observation that Python and MATLAB approximately consume the same amount of time when no optimizations are used in Python. However, we can see in the first lines of Table 1 that Python can be tuned with the C-Extensions Cython such that the execution time reaches the one of the dynamically linked C implementation, which is about 40 times faster than the plain Python or MATLAB implementation.
| Rank | Time in s | Language          | Variant          |
|------|-----------|-------------------|------------------|
|      |           |                   | Option 1 | Option 2 | Option 3|
| 1    | 0.055     | C                 | (a)      | –       | –       |
| 2    | 0.076     | C                 | (b)      | –       | –       |
| 3    | 0.077     | Python/Cython     | (b)      | (c)     | (c)     |
| 4    | 0.077     | Python/Cython     | (a)      | (c)     | (c)     |
| 5    | 1.283     | Python/Cython     | (a)      | (c)     | (b)     |
| 6    | 1.323     | Python/Cython     | (a)      | (b)     | (c)     |
| 7    | 1.337     | Python/Cython     | (b)      | (b)     | (c)     |
| 8    | 1.598     | Python/Cython     | (b)      | (c)     | (b)     |
| 9    | 2.124     | Python/Cython     | (a)      | (b)     | (b)     |
| 10   | 2.298     | Python/Cython     | (b)      | (a)     | (c)     |
| 11   | 2.426     | Python/Cython     | (b)      | (a)     | (b)     |
| 12   | 2.553     | Python/Cython     | (b)      | (c)     | (a)     |
| 13   | 2.862     | Python/Cython     | (b)      | (b)     | (b)     |
| 14   | 2.941     | Python             | (a)      | (a)     | (a)     |
| 15   | 2.973     | MATLAB             | (b)      | –       | –       |
| 16   | 3.018     | MATLAB             | (a)      | –       | –       |
| 17   | 3.359     | Python/Cython     | (b)      | (b)     | (a)     |
| 18   | 3.715     | Python             | (b)      | (a)     | (a)     |
| 19   | 4.181     | MATLAB             | (c)      | –       | –       |
| 20   | 6.590     | MATLAB             | (d)      | –       | –       |
| 21   | 112.154   | Octave             | (d)      | –       | –       |
| 22   | 133.725   | Octave             | (c)      | –       | –       |
| 23   | 138.603   | Octave             | (b)      | –       | –       |
| 24   | 152.452   | Octave             | (a)      | –       | –       |

Table 1: Execution time in seconds for $10^7$ function calls. The variants are described in Section 2.

The possibility to write performance-critical parts in the Python-like Cython syntax is a clear advantage over MATLAB and Octave because currently an optimization of function calls in MATLAB can only be achieved by writing .mex-files that require a complete rewrite of the code in another language and are often hard to handle – especially if several versions of MATLAB and thus the mex-API are used. However, we want to point out that in principle the performance of the C variants can be achieved with mex-based implementations by calling C code in the mex-files.

The Cython approach requires less effort since the Cython syntax is very similar to the plain Python syntax. Thus optimizations can be implemented easily with Cython where they are needed while maintaining the full flexibility of Python.
References

[1] R. Bradshaw et al. *The Cython compiler*. Feb. 2012. URL: http://cython.org.

[2] André Gaul. *Funcall git repository*. Feb. 2012. URL: https://bitbucket.org/andrenarchy/funcall.

[3] Eric Jones, Travis Oliphant, Pearu Peterson, et al. *SciPy: Open source scientific tools for Python*. 2001-. URL: http://www.scipy.org/.