Pythran – C++ for Snakes

Static Compiler for High Performance

Serge Guelton & Pierrick Brunet & Mehdi Amini

PyData - May 4th 2014

Get the slides: http://goo.gl/6dgra0

Disclaimer

All timings were performed using OSX 10.9, an i7-3740QM CPU @ 2.70GHz, Python 2.7.6, current Pythran (c7de8b9c), pypy 2.2.1, numba 0.13.1, gcc 4.8, Clang r207887.

I am **not** Pythonista, but I'm interested in performance in general. Daily job: driver-level C code, assembly, multi-threaded C++, GPU, ...

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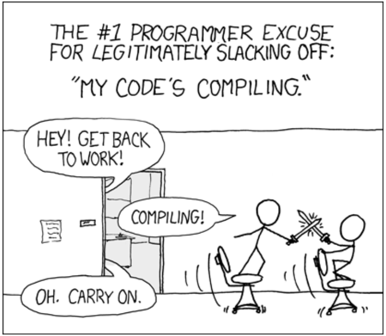

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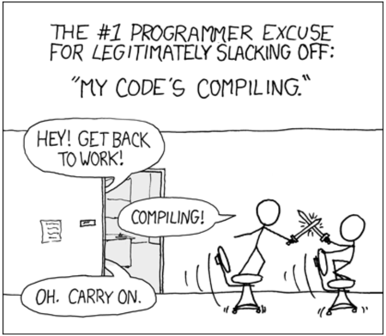

By the way this talk is written in Latex and takes more than 10 seconds to **compile**.

Prototyping Tools for Scientific Computing

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Tools for Scientific Computing in Python

theano

Cython

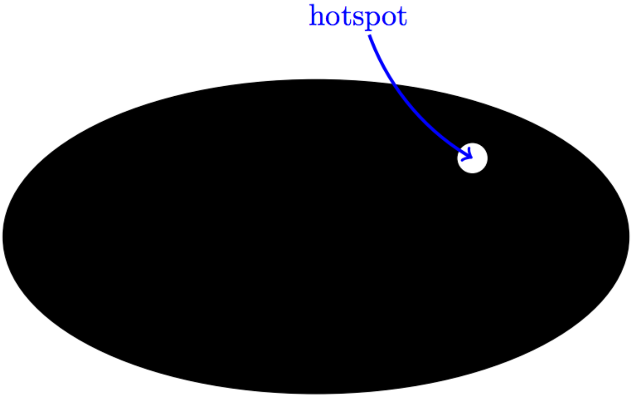
FORTRAN + f2py

NUMBA

pypy

C + SWIG

I Do not Know Much About Python But it Does not Matter Because...



I only care about the white spot.

Regular IPython Session

```
>>> import numpy as np
>>> def rosen(x):
...     return sum(100.*(x[1:]-x[:-1]**2.)**2.
...             + (1-x[:-1])**2.)
>>> import numpy as np
>>> r = np.random.rand(100000)
>>> %timeit rosen(r)
10 loops, best of 3: 35.1 ms per loop
```

In mathematical optimization, the Rosenbrock function is a non-convex function used as a performance test problem for optimization algorithms introduced by Howard H. Rosenbrock in 1960.[1] It is also known as Rosenbrock's valley or Rosenbrock's banana function. (Wikipedia)

IPython Session with Pythran

```
>>> %load_ext pythranmagic
>>> %%pythran
import numpy as np
#pythran export rosen(float[])
def rosen(x):
    return sum(100.*(x[1:]-x[:-1]**2.)**2.
          + (1-x[:-1])**2.)
>>> import numpy as np
>>> r = np.random.rand(100000)
>>> %timeit rosen(r)
10000 loops, best of 3: 121 us per loop
```

IPython Session with Pythran

```
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>>> %%pythran
import numpy as np
#pythran export rosen(float[])
def rosen(x):
     return sum(100.*(x[1:]-x[:-1]**2.)**2.
        + (1-x[:-1])**2.)
>>> import numpy as np
>>> r = np.random.rand(100000)
>>> %timeit rosen(r)
10000 loops, best of 3: 121 us per loop
```
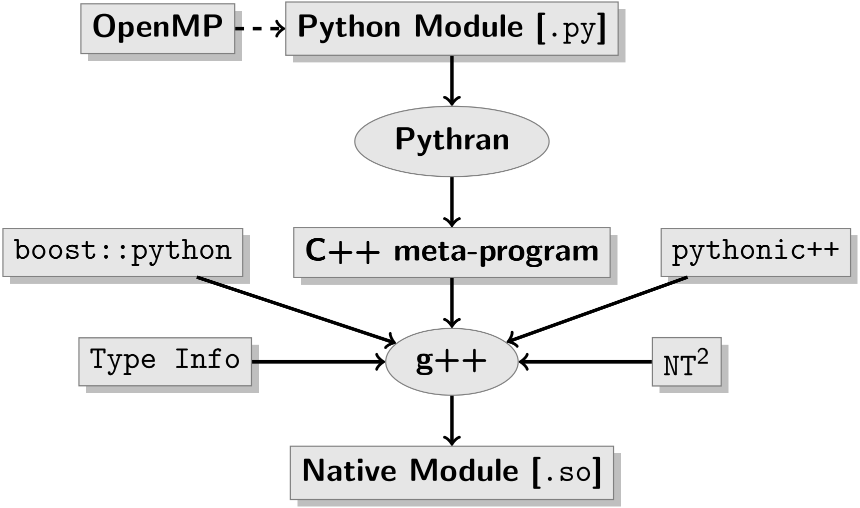

That's a $\times 290$ speedup!

Pythran's Meta Program Generator



Pythran Moto

Goals

1. Performance First
   sacrifice language feature
2. Subset of Python
   backward compatibility matters
   pythran $\approx$ python - useless stuff
   (i.e. class, eval, introspection, polymorphic variable)
3. Modular Compilation
   focus on numerical kernels

Means

1. Static Compilation
2. Static Optimizations
3. Vectorization & Parallelization

A Story of Python & C++

```python
def dot(l0, l1):
        return sum(x*y for x,y in zip(l0,l1))
```

$$\simeq$$

```cpp
template<class T0, class T1>
auto dot(T0&& l0, T1&& l1)
-> decltype(/* ... */)
{
  return pythonic::sum(
    pythonic::map(
      operator_::multiply(),
        pythonic::zip(std::forward<T0>(l0),
                      std::forward<T1>(l1))
    ) );
}
```

C++ as a Back-end

A High Level Language

- Rich Standard Template Library
- Object Oriented Programming
- Meta-Programming
- Glimpses of type inference C++11
- Variadic Templates C++11

A Low Level Language

- Few Hidden Costs: "you don't pay for what you don't use"
- Direct access to vector instruction units SSE, AVX, ...
- Good for Parallel Programming OpenMP, TBB, ...

(and the parallel STL is proposed for C++17)

Let's Dive Into the Backend Runtime...

```
template <class Op, class S0, class... Iters>
  auto map_aux (Op &op, S0 const &seq, Iters... iters)
    -> sequence <decltype(op(*seq.begin(), *iters...))>
  {
    decltype(_map(op, seq, iters...)) s;
    auto iter = std::back_inserter(s);
    for(auto& iseq : seq)
      *iter ++= op(iseq , *iters++...);
    return s;
  }
template <class Op, class S0, class... SN>
  auto map ( Op op, S0 const &seq, SN const &... seqs )
    -> decltype(_map( op, seq, seqs.begin ()...))
  {
    return _map(op, seq, seqs.begin()...);
  }
```

Let's Dive Into the Backend Runtime... I'm Kidding!

```
template <class Op, class S0, class... Iters>
  auto map_aux (Op &op, S0 const &seq, Iters... iters)
    -> sequence <decltype(op(*seq.begin(), *iters...))>
  {
    decltype(_map(op, seq, iters...)) s;
    auto iter = std::back_inserter(s);
    for(auto& iseq : seq)
      *iter ++= op(iseq , *iters++...);
    return s;
  }
template <class Op, class S0, class... SN>
  auto map ( Op op, S0 const &seq, SN const &... seqs )
    -> decltype(_map( op, seq, seqs.begin ()...))
  {
    return _map(op, seq, seqs.begin()...);
  }
```

Static Compilation

Buys time for many time-consuming analyse

Points-to, used-def, variable scope, memory effects, function purity...

Unleashes powerful C++ optimizations

Lazy Evaluation, Map Parallelizations, Constant Folding

Requires static type inference

```
#pythran export foo(int list, float)
```

Only annotate exported functions!

Pythran's Moto **1/3**

Gather as many information as possible

(Typing is just one information among others)

Example of Analysis: Points-to

```python
def foo(a,b):
    c = a or b
    return c*2
```

Where does c points to ?

Example of Analysis: Argument Effects

```
def fib(n):
    return n if n<2 else fib(n-1) + fib(n-2)

def bar(l):
    return map(fib, l)

def foo(l):
    return map(fib, random.sample(l, 3))
```

Do `fibo`, `bar` and `foo` update their arguments?

Example of Analysis: Pure Functions

```
def f0(a):
    return a**2

def f1(a):
    b = f0(a)
    print b
    return b

l = list(...)
map(f0, l)
map(f1, l)
```

Are `f0` and `f1` pure functions?

Example of Analysis: Use - Def Chains

```
a = '1'
if cond:
    a = int(a)
else:
    a = 3
print a
a = 4
```

Which version of a is seen by the print statement?

Pythran's Moto **2/3**

Gather as many information as possible

Turn them into Code Optimizations!

Example of Code Optimization: False Polymorphism

```
a = cos(1)
if cond:
    a = str(a)
else:
    a = None
foo(a)
```

Is this code snippet statically typable?

Example of Code Optimization: Lazy Iterators

```python
def valid_conversion(n):
    l = map(math.cos, range(n))
    return sum(l)

def invalid_conversion(n):
    l = map(math.cos, range(n))
    l[0] = 1
    return sum(l) + max(l)
```

Which `map` can be converted into an `imap`

Example of Code Optimization: Constant Folding

```
def esieve(n):
    candidates = range(2, n+1)
    return sorted(
        set(candidates) - set(p*i
                                for p in candidates
                                for i in range(p, n+1))
        )

cache = esieve(100)
```

Can we evalute `esieve` at compile time?

Pythran's Moto **3/3**

Gather as many information as possible

Turn them into Code Optimizations

Vectorize! Parallelize!

Explicit Parallelization

```
def hyantes(xmin, ymin, xmax, ymax, step, range_, range_x, range_y, t):
  pt = [[0]*range_y for _ in range(range_x)]
  "omp␣parallel␣for"
  for i in xrange(range_x):
    for j in xrange(range_y):
      s = 0
      for k in t:
        tmp = 6368.* math.acos(math.cos(xmin+step*i)*math.cos( k[0] ) *
                               math.cos((ymin+step*j)-k[1]) +
                               math.sin(xmin+step*i)*math.sin(k[0]))
        if tmp < range_:
          s+=k[2] / (1+tmp)
      pt[i][j] = s
  return pt
```

Tool	CPython	Pythran	OpenMP
Timing	639.0ms	44.8ms	11.2ms
Speedup	$\times 1$	$\times 14.2$	$\times 57.7$

Library Level Optimizations

Numpy is the key

- Basic block of Python Scientific Computing
- High-level Array Manipulations
- Many common functions implemented

1. This smells like FORTRAN
2. For the compiler guy, FORTRAN smells good
3. Unlock vectorization & parallelization of Numpy code!

Cython is known to be "as fast as C", the only way we found to beat it is to be "as fast as Fortran", hence: Py**thran**

Efficient Numpy Expressions

Expression Templates

1. A classic C++ meta-programming optimization
2. Brings Lazy Evaluation to C++
3. Equivalent to loop fusion

More Optimizations

- vectorization through `boost::simd` and `nt2`
- parallelization through `#pragma omp`

Julia Set, a Cython Example

```
def run_julia(cr, ci, N, bound, lim, cutoff):
    julia = np.empty((N, N), np.uint32)
    grid_x = np.linspace(-bound, bound, N)
    t0 = time()
    "omp␣parallel␣for"
    for i, x in enumerate(grid_x):
        for j, y in enumerate(grid_x):
            julia[i,j] = kernel(x, y, cr, ci, lim, cutoff)
    return julia, time() - t0
```

From Scipy2013 Cython Tutorial.

Tool	CPython	Cython	Pythran	+OpenMP
Timing	3630ms	4.3ms	3.71ms	1.52ms
Speedup	×1	×837	×970	×2368

Mandelbrot, a Numba example

```python
@autojit
def mandel(x, y, max_iters):
    """
    Given the real and imaginary parts of a complex
    determine if it is a candidate for membership in
    set given a fixed number of iterations.
    """
    i = 0
    c = complex(x, y)
    z = 0.0j
    for i in range(max_iters):
        z = z**2 + c
        if abs(z)**2 >= 4:
            return i

    return 255
```

```python
@autojit
def create_fractal(min_x, max_x, min_y, max_y, image, iters)
    height = image.shape[0]
    width = image.shape[1]

    pixel_size_x = (max_x - min_x) / width
    pixel_size_y = (max_y - min_y) / height

    for x in range(width):
        real = min_x + x * pixel_size_x
        for y in range(height):
            imag = min_y + y * pixel_size_y
            color = mandel(real, imag, iters)
            image[y, x] = color

    return image
```

Tool	CPython	Numba	Pythran
Timing	8170ms	56ms	83ms
Speedup	×1	×145	×98

Nqueens, to Show Some Cool Python

```python
# Pure-Python implementation of
# itertools.permutations()
# Why? Because we can :-)
def permutations(iterable, r=None):
  pool = tuple(iterable)
  n = len(pool)
  if r is None:
    r = n
  indices = range(n)
  cycles = range(n-r+1, n+1)[::-1]
  yield tuple(pool[i] for i in indices[:r])
  while n:
    for i in reversed(xrange(r)):
      cycles[i] -= 1
      if cycles[i] == 0:
        indices[i:] = indices[i+1:] + indices[i:i+1]
        cycles[i] = n - i
      else:
        j = cycles[i]
        indices[i], indices[-j] = \
            indices[-j], indices[i]
        yield tuple(pool[i] for i in indices[:r])
        break
    else:
      return
```

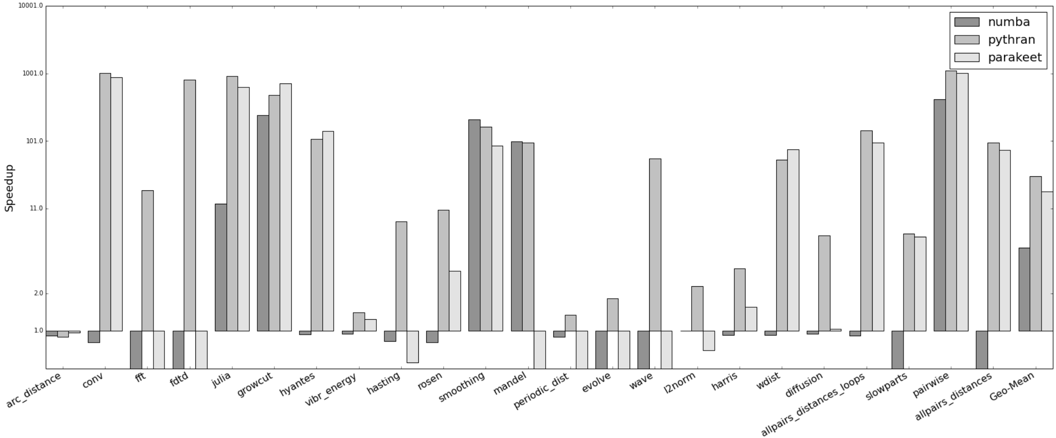
```python
#pythran export n_queens(int)
def n_queens(queen_count):
  """N-Queens solver.
  Args:
    queen_count: the number of queens to solve
    for. This is also the board size.

  Yields:
    Solutions to the problem. Each yielded
    value is looks like (3, 8, 2, ..., 6)
    where each number is the column position
    for the queen, and the index into the
    tuple indicates the row.
  """
  out =list()
  cols = range(queen_count)
  for vec in permutations(cols,None):
    if (queen_count == len(set(vec[i]+i
                               for i in cols))):
      out.append(vec)
  return out
```

Solving the NQueen problem, using generator, generator expression, list comprehension, sets. . .

http://code.google.com/p/unladen-swallow/

Tool	CPython	PyPy	Pythran
Timing	2640.6ms	501.1ms	693.3ms
Speedup	×1	×5.27	×3.8

Numpy Benchmarks

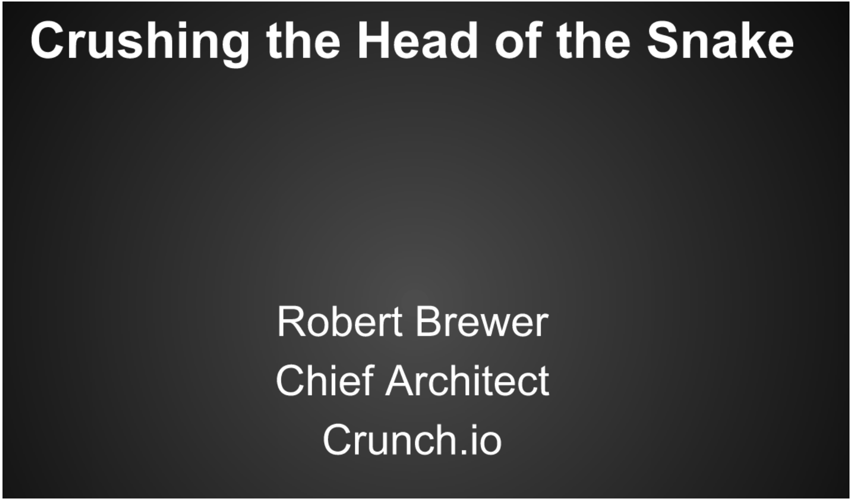


https://github.com/serge-sans-paille/numpy-benchmarks/

Made with Matplotlib last night!

Debian clang version 3.5-1 exp1, x86-64, i7-3520M CPU @ 2.90GHz. No OpenMP/Vectorization for Pythran.

Crushing the Head of the Snake



I would have titled it "What every Pythonista should know about Python!"

(hopefully we'll get the video soon).

The Compiler Is not the Solution to Keyboard-Chair Interface, Is It?

```python
def total(arr):
    s = 0
    for j in range(len(arr)):
        s += arr[j]
    return s


def varsum(arr):
    vs = 0
    for j in range(len(arr)):
        mean = (total(arr) / len(arr))
        vs += (arr[j] - mean) ** 2
    return vs
```

```python
#pythran export stddev(float64 list list)
def stddev(partitions):
    ddof=1
    final = 0.0
    for part in partitions:
        m = total(part) / len(part)
        # Find the mean of the entire grup.
        gtotal = total([total(p) for p in partitions])
        glength = total([len(p) for p in partitions])
        g = gtotal / glength
        adj = ((2 * total(part) * (m - g)) + ((g ** 2 - m **
        final += varsum(part) + adj
    return math.sqrt(final / (glength - ddof))
```

Version	Awful	Less Awful	OK	*Differently OK*	*OK*	Numpy
CPython	127s	150ms	54.3ms	53.8ms	47.6ms	8.2ms
Pythran	1.38s	4.7ms	4.8ms	5.8ms	4.7ms	1.7ms

Engineering Stuff

Get It

- Follow the source: `https://github.com/serge-sans-paille/pythran`
  (we are waiting for your pull requests)
- Debian repo: `deb http://ridee.enstb.org/debian unstable main`
- Join us: `#pythran` on Freenode *(very active)*,
  or `pythran@freelists.org` *(not very active)*

Available on PyPI, using Python 2.7, +2000 test cases, PEP8 approved, clang++ & g++ (>= 4.8) friendly, Linux and OSX validated.

Conclusions

http://pythonhosted.org/pythran/

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- More Numpy support, start looking into Scipy
- Polyhedral transformations (for my next life...)