Pythran: Static Compilation of Parallel Scientific Kernels

a.k.a. Python/Numpy compiler for the mass

Proudly made in *Namek* by serge-sans-paille & pbrunet

/us

Serge « sans paille » Guelton

```
$ whoami
sguelton
```

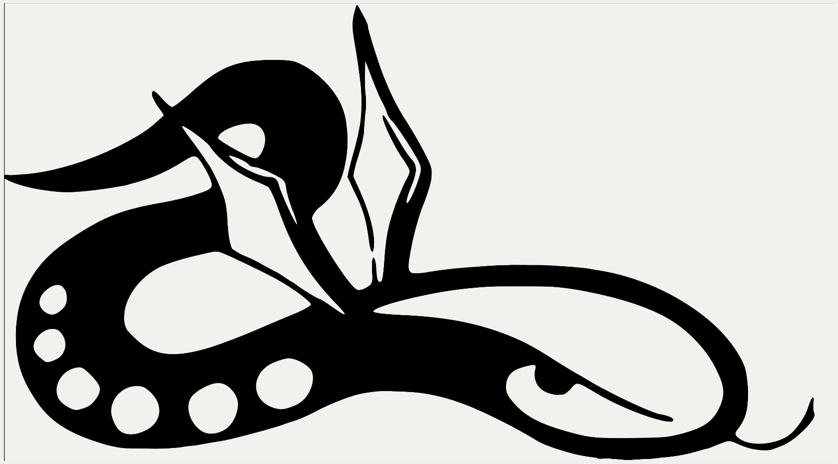
- R&D engineer at QuarksLab on compilation for security
- Associate researcher at Télécom Bretagne

Pierrick Brunet

```
$ whoami
pbrunet
```

- R&D engineer at INRIAlpes/MOAIS on parallelism

Pythran in a snake shell



- A Numpy-centric Python-to-C++ translator
- A Python code *optimizer*
- A Pythonic C++ library

Core concepts

- Focus on high-level constructs
- Generate ~~clean~~ high level code
- Optimize Python code before generated code
- Vectorization and Paralllelism
- Test, test, test
- Bench, bench, bench

Ask StackOverflow

when you're looking for ***test cases***

http://stackoverflow.com/[...]numba-or-cython-acceleration-in-reaction-diffusion-algorithm

```
import numpy as np
def GrayScott(counts, Du, Dv, F, k):
    n = 300
    U = np.zeros((n+2,n+2), dtype=np.float32)
    V = np.zeros((n+2,n+2), dtype=np.float32)
    u, v = U[1:-1,1:-1], V[1:-1,1:-1]

    r = 20
    u[:] = 1.0
    U[n/2-r:n/2+r,n/2-r:n/2+r] = 0.50
    V[n/2-r:n/2+r,n/2-r:n/2+r] = 0.25
    u += 0.15*np.random.random((n,n))
    v += 0.15*np.random.random((n,n))

    for i in range(counts):
        Lu = (                 U[0:-2,1:-1] +
              U[1:-1,0:-2] - 4*U[1:-1,1:-1] + U[1:-1,2:] +
                               U[2:  ,1:-1] )
```

Thread Summary

OP

My code is slow with Cython and Numba

Best Answer

You need to make all loops explicit

Cython Version

```
cimport cython
import numpy as np
cimport numpy as np

cpdef cythonGrayScott(int counts, double Du, double Dv, double F, double
    cdef int n = 300
    cdef np.ndarray U = np.zeros((n+2,n+2), dtype=np.float_)
    cdef np.ndarray V = np.zeros((n+2,n+2), dtype=np.float_)
    cdef np.ndarray u = U[1:-1,1:-1]
    cdef np.ndarray v = V[1:-1,1:-1]

    cdef int r = 20
    u[:] = 1.0
    U[n/2-r:n/2+r,n/2-r:n/2+r] = 0.50
    V[n/2-r:n/2+r,n/2-r:n/2+r] = 0.25
    u += 0.15*np.random.random((n,n))
    v += 0.15*np.random.random((n,n))
```

Pythran version

Add this line to the original kernel:

```
#pythran export GrayScott(int, float, float, float, float)
```

Timings

```
$ python -m timeit -s 'from grayscott import GrayScott' 'GrayScott(40, 0
10 loops, best of 3: 52.9 msec per loop
$ cython grayscott.pyx
$ gcc grayscott.c `python-config --cflags --libs` -shared -fPIC -o grays
$ python -m timeit -s 'from grayscott import GrayScott' 'GrayScott(40, 0
10 loops, best of 3: 36.4 msec per loop
$ pythran grayscott.py -O3 -march=native
$ python -m timeit -s 'from grayscott import GrayScott' 'GrayScott(40, 0
10 loops, best of 3: 20.3 msec per loop
```

Lessons learnt

- Explicit is not always better than implicit
- Many ``optimization hints'' can be deduced by the compiler
- High level constructs carry valuable informations

*I am **not** saying Cython is bad. Cython does a **great** job. It is just **pragmatic** where Pythran is **idealist***

Compilation Challenges

```
u = U[1:-1,1:-1]
U[n/2-r:n/2+r,n/2-r:n/2+r] = 0.50
u += 0.15*np.random.random((n,n))
```

- Array views
- Value broadcasting
- Temporary arrays creation
- Extended slices composition
- Numpy API calls

Optimization Opportunities

```
Lu = (U[0:-2,1:-1] + U[1:-1,0:-2]
  - 4*U[1:-1,1:-1] + U[1:-1,2:] + U[2:  ,1:-1])
```

- Many useless temporaries
- `Lu` could be forward-substituted
- SIMD instruction generation opportunities
- Parallel loop opportunities

Pythran Usage

```
$ pythran --help
usage: pythran [-h] [-o OUTPUT_FILE] [-E] [-e] [-f flag] [-v] [-p pass]
               [-m machine] [-I include_dir] [-L ldflags]
               [-D macro_definition] [-O level] [-g]
               input_file

pythran: a python to C++ compiler

positional arguments:
  input_file           the pythran module to compile, either a .py or a
                       file

optional arguments:
  -h, --help           show this help message and exit
  -o OUTPUT_FILE       path to generated file
  -E                   only run the translator, do not compile
  -e                   similar to -E, but does not generate python glue
  -f flag              any compiler switch relevant to the underlying C+
```

Sample Usage

```
$ pythran input.py # generates input.so
$ pythran input.py -E # generates input.cpp
$ pythran input.py -O3 -fopenmp # parallel!
$ pythran input.py -march=native -Ofast # Esod Mumixam !
```

Type Annotations

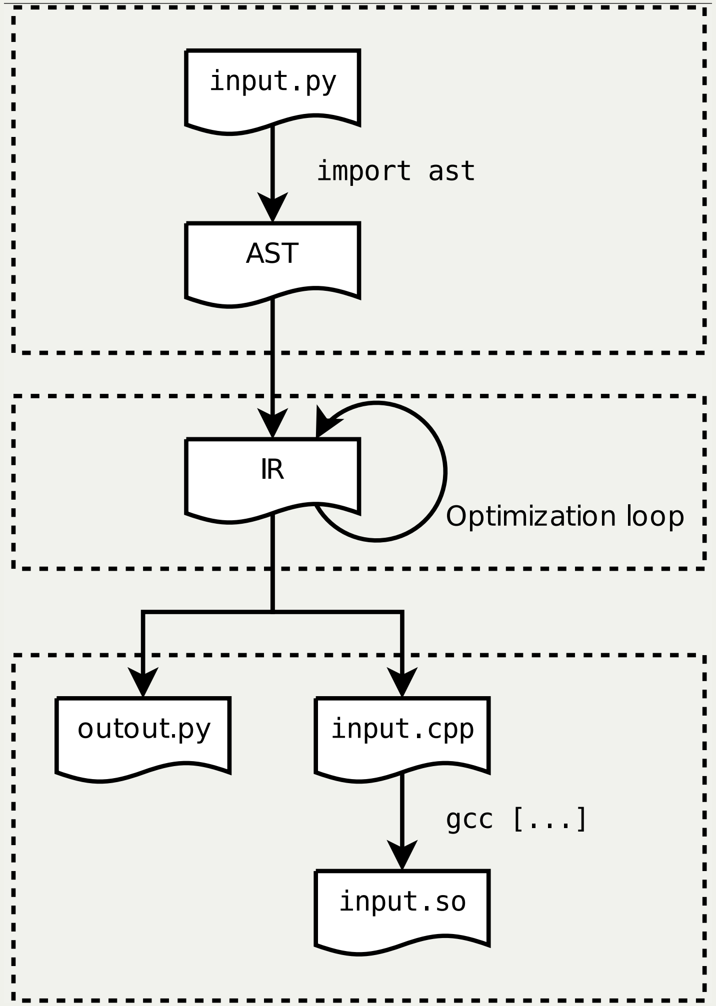
Only for *exported* functions

```
#pythran export foo0()
#pythran export foo1(int)

#pythran export foo2(float32[][])
#pythran export foo2(float64[][])
#pythran export foo2(int8[][][])

#pythran export foo3((int, float), int list, str:str dict)
```

Pythran Compilation Flow



Front End

- 100% based on the `ast` module
- Supports
  - Several standard module (incl. partial Numpy)
  - Polymorphic functions
  - ndarray, list, tuple, dict, str, int, long, float
  - Named parameters, default arguments
  - Generators…
- Does not Support
  - Non-implicitely typed code
  - Global variable
  - Most Python modules (no CPython mode!)
  - User-defined classes…

Middle End

Iteratively applies high level, Python-aware optimizations:

- Interprocedural Constant Folding
- For-Based-Loop Unrolling
- Forward Substitution
- Instruction Selection
- Deforestation
- Scalar Renaming
- dead Code Elimination

Fun Facts: can evaluate pure functions at compile time ☺

Back Ends

Python Back End

Useful for debugging!

C++11 Back End

- C++11 implementation of `__builtin__` `numpy` `itertools`…
- Lazy evaluation through Expression Templates
- Relies on OpenMP, `nt2` and `boost::simd` for the parallelization / vectorization

C++11: Typing

the W.T.F. slide

Pythran translates Python implicitly statically typed **polymorphic** code into C++ **meta-programs** that are instanciated for the user-given types, and specialize them for the target architecture

C++11: Parallelism

Implicit

Array operations and several numpy functions are written using OpenMP and Boost.simd

Explicit

OpenMP 3 support, ported to Python

```
#omp parallel for reduction(+:r)
for i, v in enumerate(l):
    r += i * v
```

Benchmarks

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

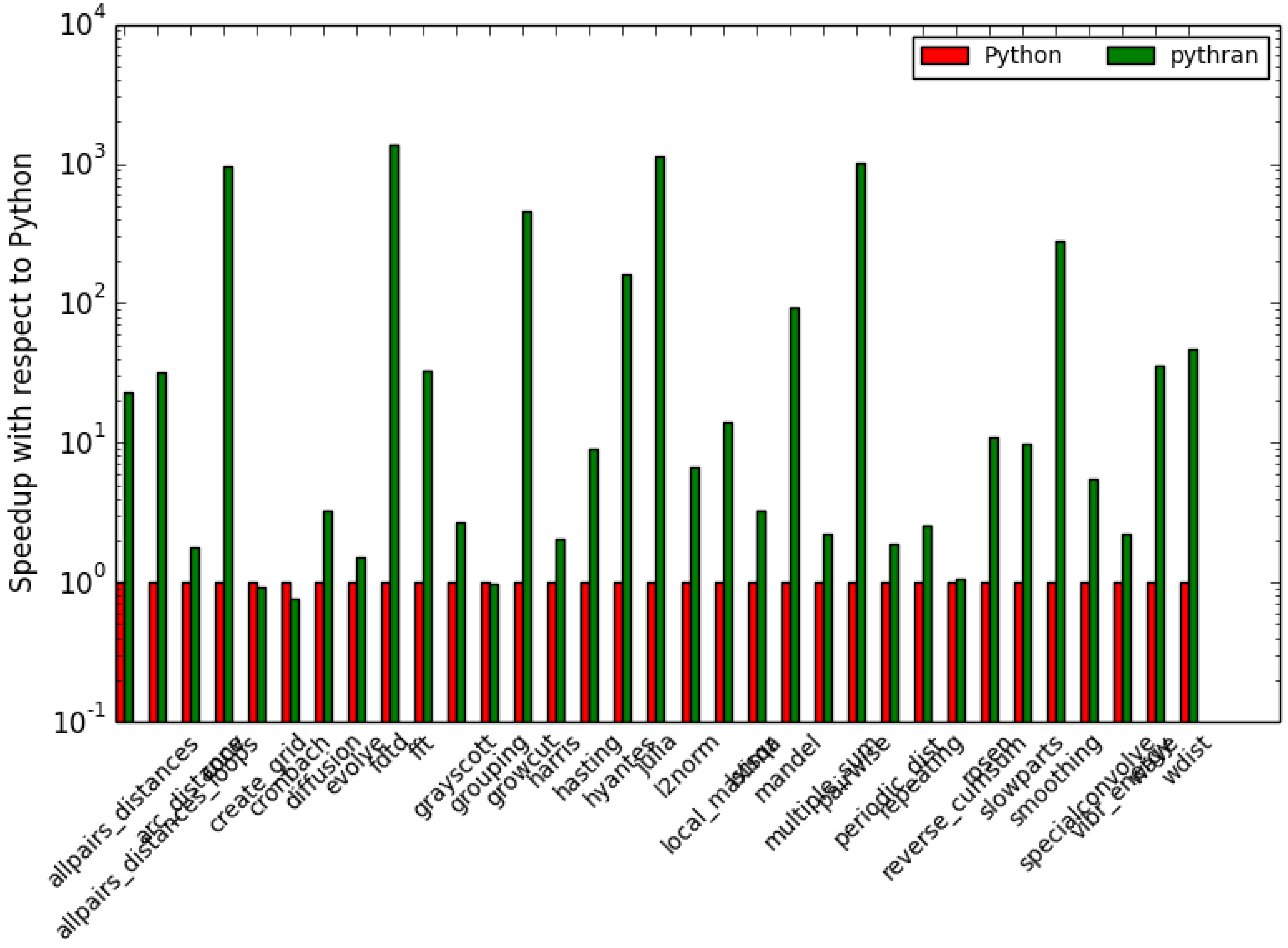
A collection of high-level benchmarks

- Code gathered from StackOverflow + other compiler code base
- Mostly high-level code
- Generate results for CPython, PyPy, Numba, Parakeet, Hope and Pythran

Most kernels are too high level for Numba and Hope…

Benchmarks

no parallelism, no vectorisation (, no fat)


Speedup with respect to Python
Python
pythran
10^{4}
10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
allpairs_distances
allpairs_distances_loops
create_grid
cronbach
diffusion
evolve
fdtd
fft
grayscott
grouping
growcut
harris
hasting
hyantes
julia
l2norm
local_maxima
mandel
multiple_sum
pairwise
periodic_dist
repeating
reverse_cumsum
rosen
slowparts
smoothing
specialconvolve
wdist

(Num)Focus: growcut

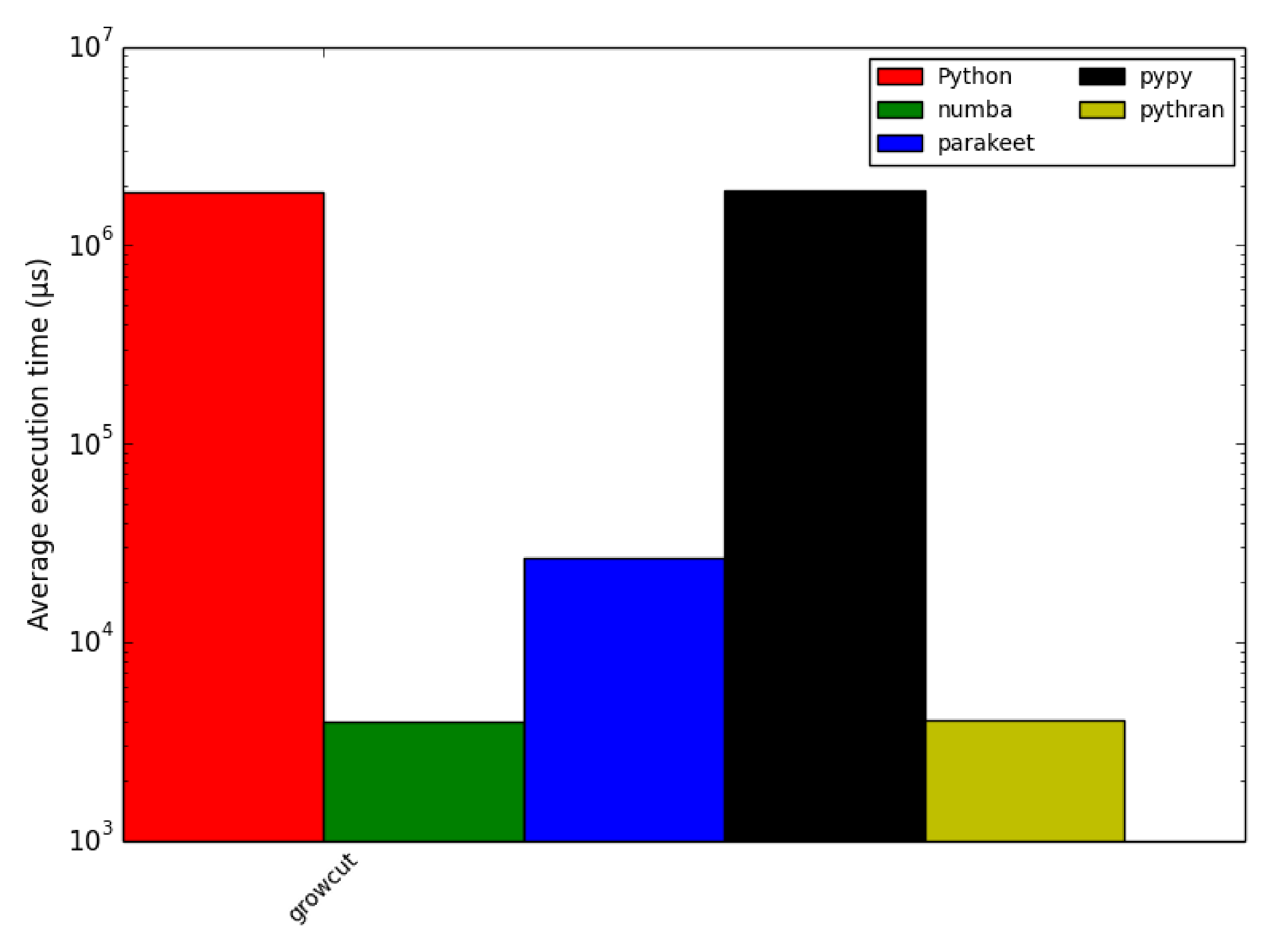
From the Numba codebase!

```
#pythran export growcut(float[][][], float[][][], float[][][], int)
import math
import numpy as np
def window_floor(idx, radius):
    if radius > idx:
        return 0
    else:
        return idx - radius


def window_ceil(idx, ceil, radius):
    if idx + radius > ceil:
        return ceil
    else:
        return idx + radius

def growcut(image, state, state_next, window_radius):
    changes = 0
```

(Num)Focus: growcut



Academic Results

- **Pythran: Enabling Static Optimization of Scientific Python Programs**, S. Guelton, P. Brunet et al. in *CSD*, 2015
- **Exploring the Vectorization of Python Constructs Using Pythran and Boost SIMD**, S. Guelton, J. Falcou and P. Brunet, in *WPMVP*, 2014
- **Compiling Python modules to native parallel modules using Pythran and OpenMP Annotations**, S. Guelton, P. Brunet and M. Amini, in *PyHPC*, 2013
- **Pythran: Enabling Static Optimization of Scientific Python Programs**, S. Guelton, P. Brunet et al. in *SciPy*, 2013

Powered by Strong Engineering

Preprequisite for reproductible science

- 2773 test cases, incl. unit testing, doctest, **Continuous integration** (thx Travis!)
- Peer-reviewed code
- Python2.7 and C++11
- Linux, OSX (almost okay), Windows (on going)
- User and Developer doc: http://pythonhosted.org/pythran/
- Hosted on https://github.com/serge-sans-paille/pythran
- Releases on PyPi: `$ pip install pythran`
- Custom Debian repo: `$ apt-get install pythran`

We need more peons

- Pythonic needs a serious cleanup
- Typing module needs better error reporting
- OSX support is partial and Windows support is on-going
- `numpy.random` and `numpy.linalg`

THE END

AUTHORS

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INDUSTRIAL SUPPORT

Silkan, NumScale, **→You←**

CONTRIBUTE

#pythran on FreeNode, pythran@freelists.org, GitHub repo