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Python Scalability Story In Production Environments

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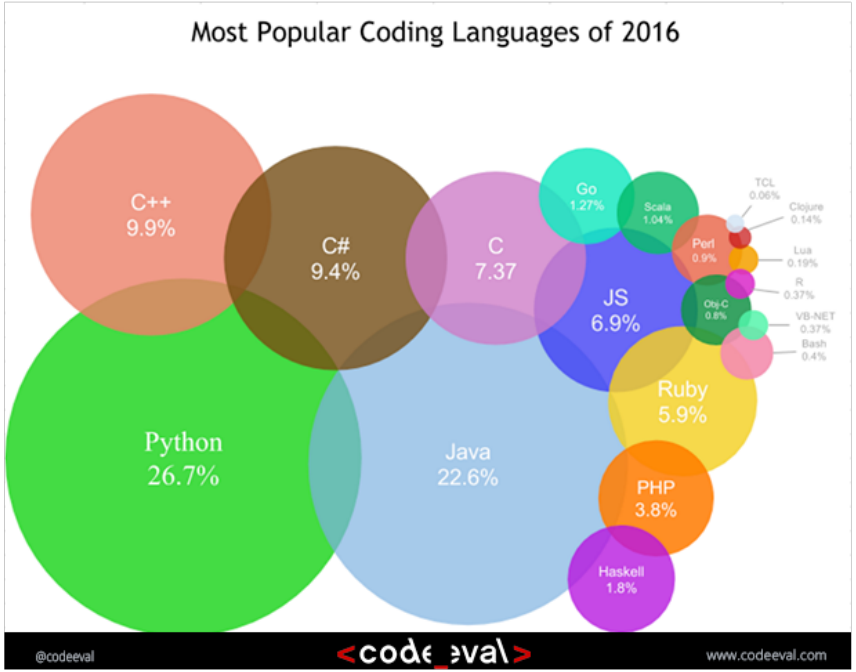
Director of Community Innovation

Continuum Analytics

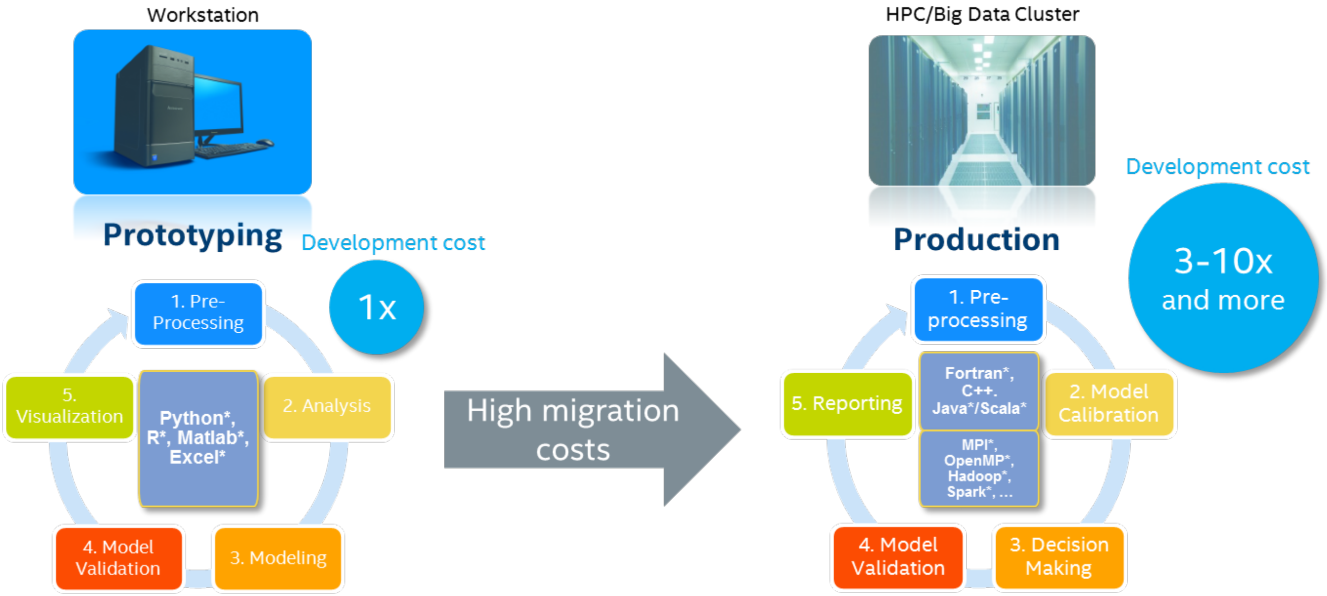
Motivation: Why Python

Python is **#1** programming language in **hiring demand** followed by **Java** and **C++**.

And the demand is **growing**

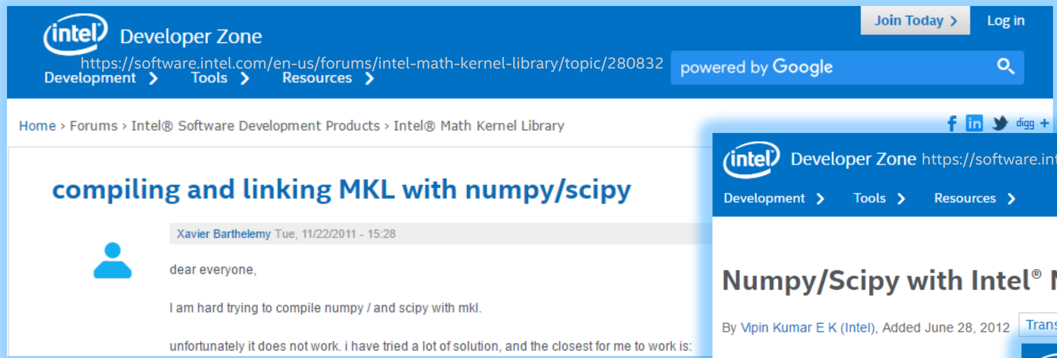


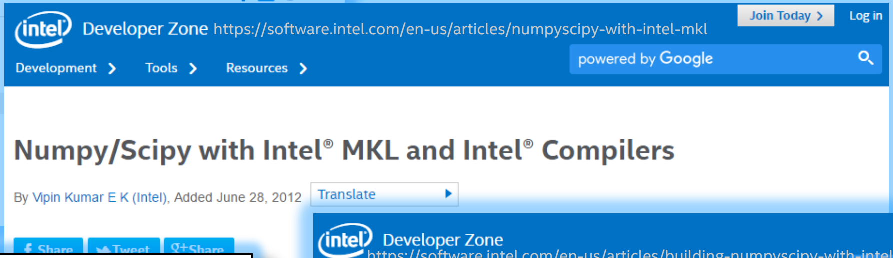
What Problems We Solve: Scalable Performance

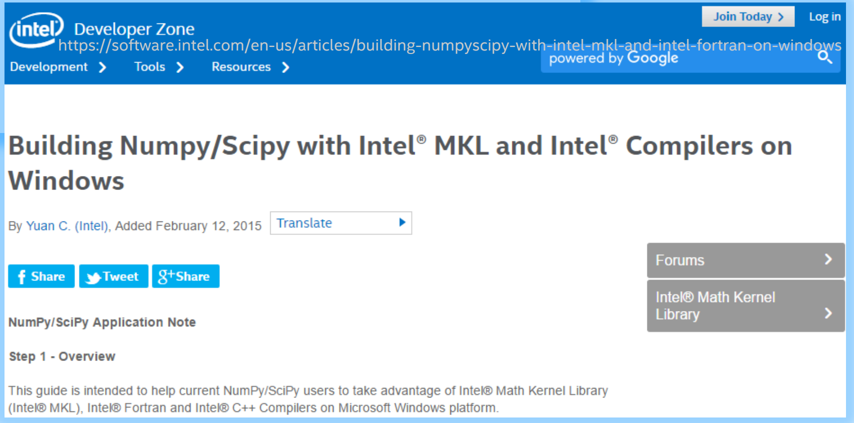


Make Python usable beyond prototyping environment by scaling out to HPC and Big Data environments

What Problems We Solve: Out-Of-The-Box Usability







"Any articles I found on your site that related to actually using the MKL for compiling something were overly technical. ***I couldn't figure out what the heck some of the things were doing or talking about****."* – Intel® Parallel Studio 2015 Beta Survey Response

INTEL® DISTRIBUTION FOR PYTHON* 2017

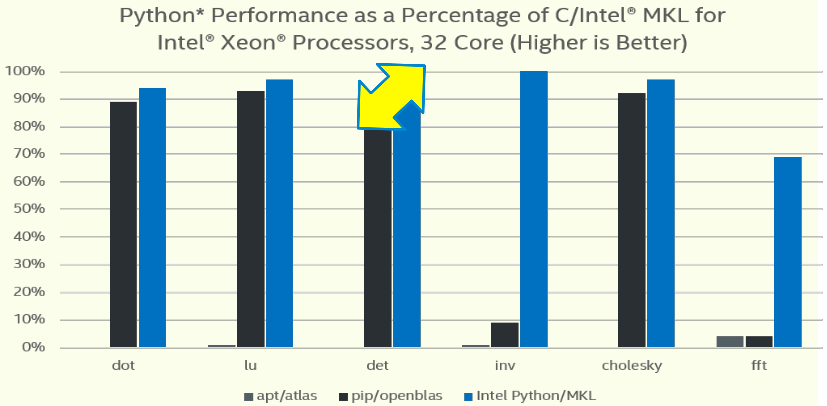
Advancing Python performance closer to native speeds

Easy, out-of-the-box access to high performance Python	• Prebuilt, optimized for numerical computing, data analytics, HPC • Drop in replacement for existing Python. No code changes required
Performance with multiple optimization techniques	• Accelerated NumPy/SciPy/Scikit-Learn with Intel® MKL • Data analytics with pyDAAL, enhanced thread scheduling with TBB, Jupyter* Notebook interface, Numba, Cython • Scale easily with optimized MPI4Py and Jupyter notebooks
Faster access to latest optimizations for Intel architecture	• Distribution and individual optimized packages available through conda and Anaconda Cloud: `anaconda.org/intel` • Optimizations upstreamed back to main Python trunk

Why Yet Another Python Distribution?

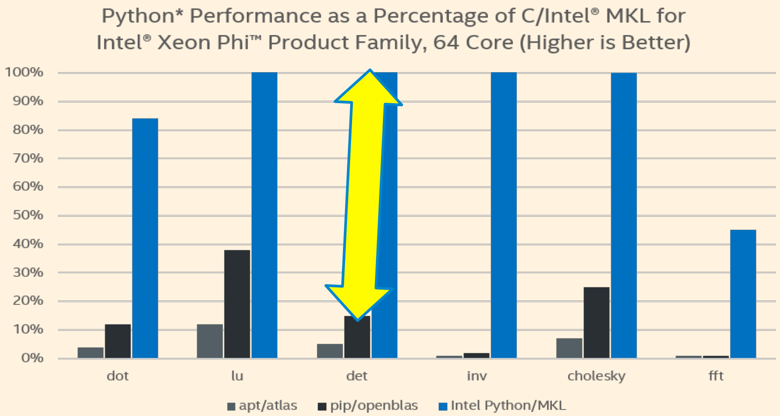
Mature AVX2 instructions based product

Intel® Xeon® Processors



New AVX512 instructions based product

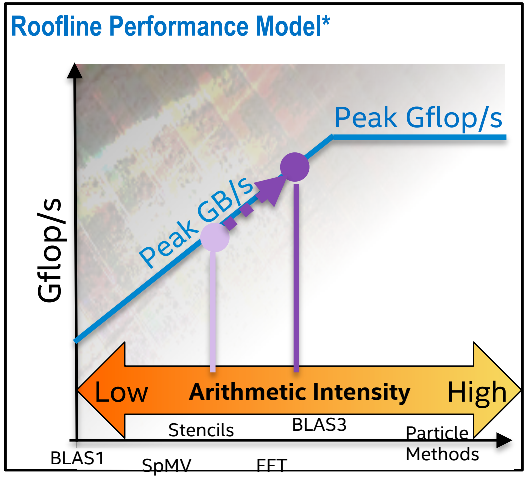
Intel® Xeon Phi™ Product Family

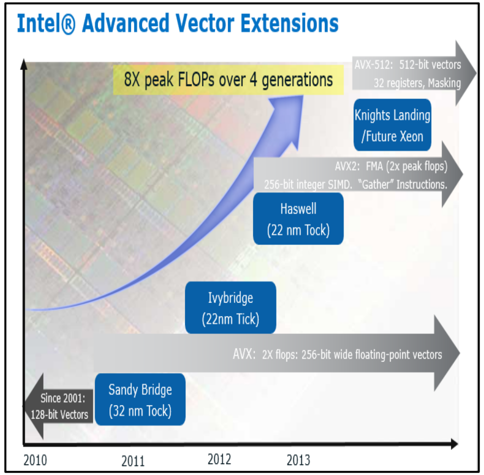


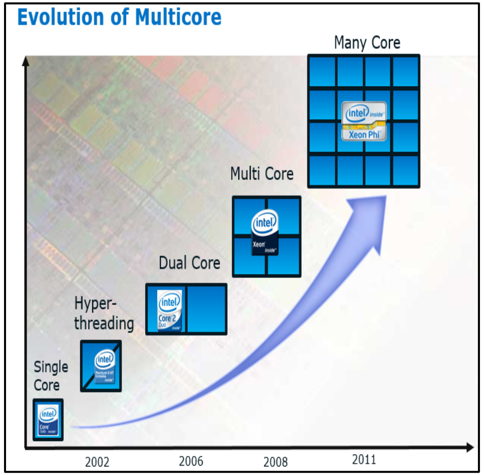
Configuration Info: apt/atlas: installed with apt-get, Ubuntu 16.10, python 3.5.2, numpy 1.11.0, scipy 0.17.0; pip/openblas: installed with pip, Ubuntu 16.10, python 3.5.2, numpy 1.11.1, scipy 0.18.0; Intel Python: Intel Distribution for Python 2017;. Hardware: Xeon: Intel Xeon CPU E5-2698 v3 @ 2.30 GHz (2 sockets, 16 cores each, HT=off), 64 GB of RAM, 8 DIMMS of 8GB@2133MHz; Xeon Phi: Intel Intel® Xeon Phi™ CPU 7210 1.30 GHz, 96 GB of RAM, 6 DIMMS of 16GB@1200MHz

Scaling To HPC/Big Data Production Environment

- Hardware and software efficiency crucial in production (Perf/Watt, etc.)
- Efficiency = Parallelism
  - Instruction Level Parallelism with effective memory access patterns
  - SIMD
  - Multi-threading
  - Multi-node







* Roofline Performance Model https://crd.lbl.gov/departments/computer-science/PAR/research/roofline/

Efficiency = Parallelism in Python

- CPython as interpreter inhibits parallelism but…
- … Overall Python tools evolved far toward unlocking parallelism

Native extensions numpy*, scipy*, scikit-learn* accelerated with Intel® MKL, Intel® DAAL, Intel® IPP

Composable multi-threading with Intel® TBB and Dask*

Multi-node parallelism with mpi4py* accelerated with Intel® MPI

Language extensions for vectorization & multi-threading (Cython*, Numba*)

Integration with Big Data platforms and Machine Learning frameworks (pySpark*, Theano*, TensorFlow*, etc.)

Mixed language profiling with Intel® VTune™ Amplifier

Numpy* & Scipy* optimizations with Intel® MKL

Configuration Info: apt/atlas: installed with apt-get, Ubuntu 16.10, python 3.5.2, numpy 1.11.0, scipy 0.17.0; pip/openblas: installed with pip, Ubuntu 16.10, python 3.5.2, numpy 1.11.1, scipy 0.18.0; Intel Python: Intel Distribution for Python 2017;. Hardware: Xeon: Intel Xeon CPU E5-2698 v3 @ 2.30 GHz (2 sockets, 16 cores each, HT=off), 64 GB of RAM, 8 DIMMS of 8GB@2133MHz; Xeon Phi: Intel Intel® Xeon Phi™ CPU 7210 1.30 GHz, 96 GB of RAM, 6 DIMMS of 16GB@1200MHz

Linear Algebra

- BLAS
- LAPACK
- ScaLAPACK
- Sparse BLAS
- Sparse Solvers
  - Iterative
  - PARDISO* SMP & Cluster

Up to 100x faster!

Fast Fourier Transforms

- 1D and multidimensional FFT

Up to 10x faster!

Vector Math

- Trigonometric
- Hyperbolic
- Exponential
- Log
- Power
- Root

Up to 10x faster!

Vector RNGs

- Multiple BRNG
- Support methods for independent streams creation
- Support all key probability distributions

Up to 60x faster!

Summary Statistics

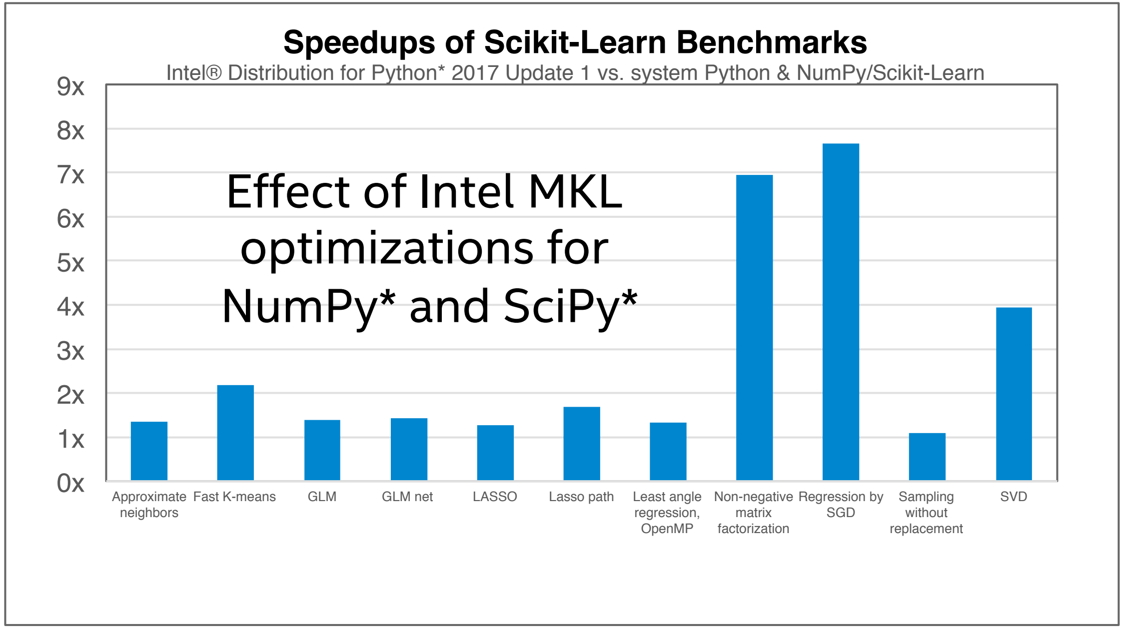
- Kurtosis
- Variation coefficient
- Order statistics
- Min/max
- Variance-covariance

And More

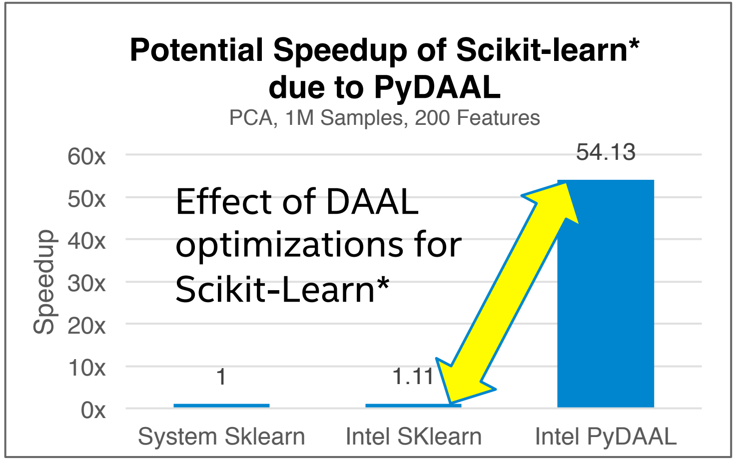
- Splines
- Interpolation
- Trust Region
- Fast Poisson Solver

Functional domain in this color accelerate respective NumPy, SciPy, etc. domain

Scikit-Learn* optimizations with Intel® MKL



Intel® Distribution for Python* ships Intel® Data Analytics Acceleration Library with Python interfaces, a.k.a. pyDAAL



System info: 32x Intel® Xeon® CPU E5-2698 v3 @ 2.30GHz, disabled HT, 64GB RAM; Intel® Distribution for Python* 2017 Gold; Intel® MKL 2017.0.0; Ubuntu 14.04.4 LTS; Numpy 1.11.1; scikit-learn 0.17.1. See Optimization Notice.

Distributed parallelism

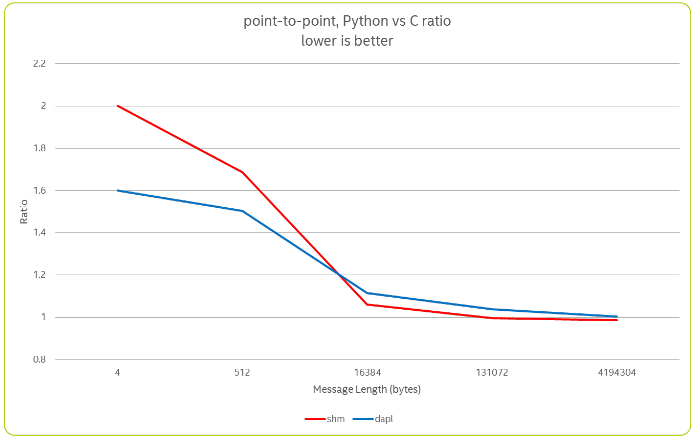
Intel® MPI library accelerates Intel® Distribution for Python* (Mpi4py*, Ipyparallel*)

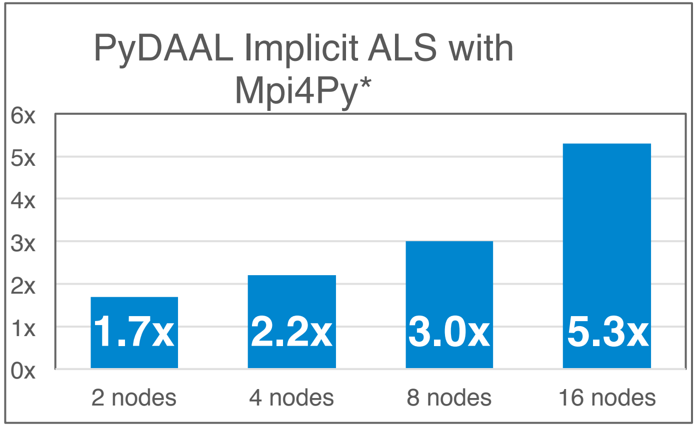
Intel Distribution for Python* also supports

- PySpark* - Python interfaces for Spark*, a fast and general engine for large-scale data processing.
- Dask* - a flexible parallel computing library for analytic computing.

Configuration Info: Intel(R) Xeon(R) CPU E5-2697 v4 @ 2.30GHz, 2x18 cores, HT is ON, RAM 128GB; Versions: Oracle Linux Server 6.6, Intel® DAAL 2017 Gold, Intel® MPI 5.1.3; Interconnect: 1 GB Ethernet

Mpi4py* performance vs. native Intel® MPI

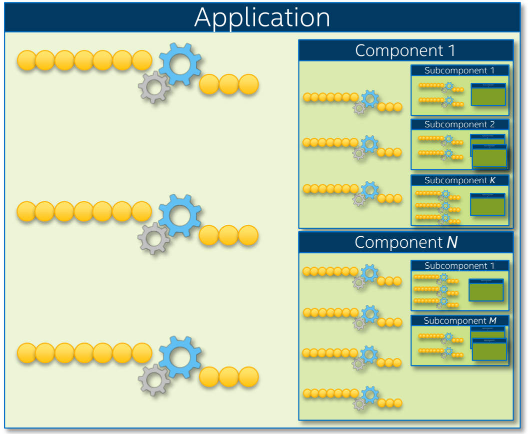


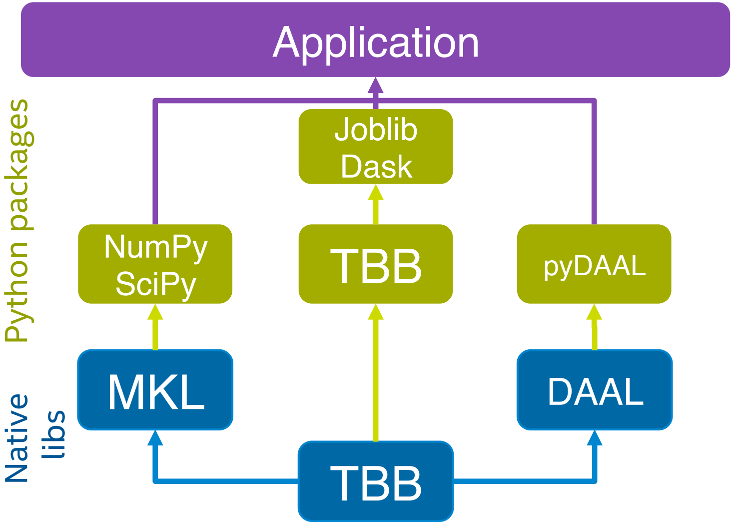


Composable multi-threading with Intel® TBB

- Amhdal's law suggests extracting parallelism at all levels
- Software components are built from smaller ones
- If each component is threaded there can be too much!
- Intel TBB dynamically balances thread loads and effectively manages oversubscription

```
>python -m TBB myapp.py
```

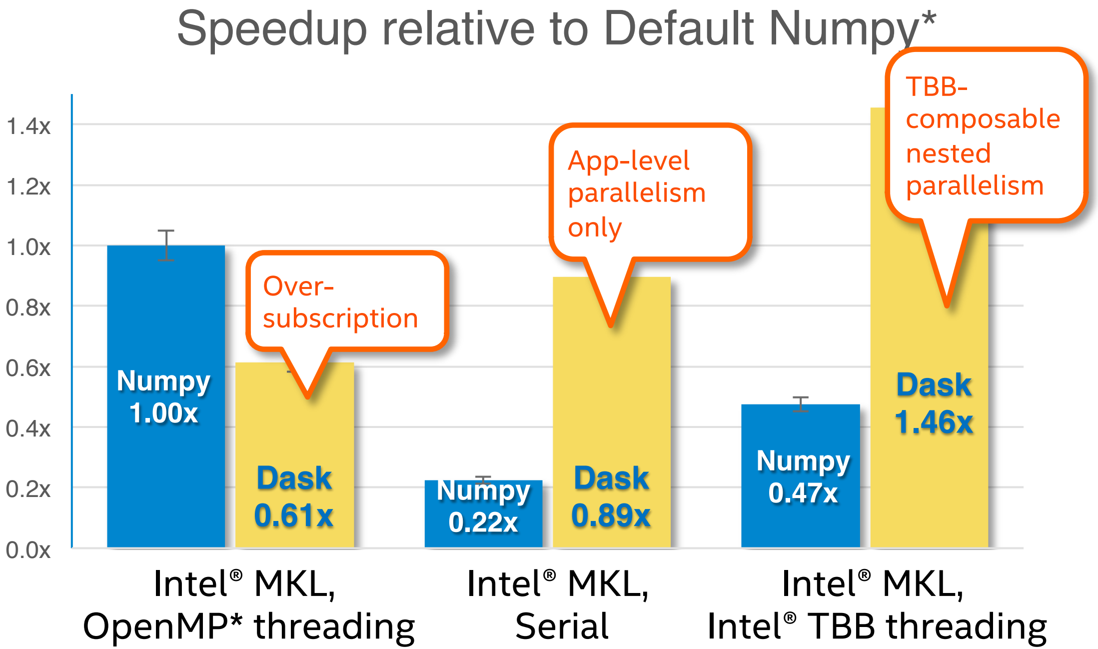




Composable Parallelism: QR Performance

```python
import time, numpy as np
x = np.random.random((100000, 2000))
t0 = time.time()
q, r = np.linalg.qr(x)
test = np.allclose(x, q.dot(r))
assert(test)
print(time.time() - t0)
```

```python
import time, dask, dask.array as da
x = da.random.random((100000, 2000),
                     chunks=(10000, 2000))
t0 = time.time()
q, r = da.linalg.qr(x)
test = da.all(da.isclose(x, q.dot(r)))
assert(test.compute()) # threaded
print(time.time() - t0)
```



System info: 32x Intel(R) Xeon(R) CPU E5-2698 v3 @ 2.30GHz, disabled HT, 64GB RAM; Intel(R) MKL 2017.0 Beta Update 1 Intel(R) 64 architecture, Intel(R) AVX2; Intel(R)TBB 4.4.4; Ubuntu 14.04.4 LTS; Dask 0.10.0; Numpy 1.11.0. Software and workloads used in performance tests may have been optimized for performance only on Intel microprocessors. Performance tests, such as SYSmark and MobileMark, are measured using specific computer systems, components, software, operations and functions. Any change to any of those factors may cause the results to vary. You should consult other information and performance tests to assist you in fully evaluating your contemplated purchases, including the performance of that product when combined with other products. * Other brands and names are the property of their respective owners. Benchmark Source: Intel Corporation

Profiling Python* code with Intel® VTune™ Amplifier

Right tool for high performance application profiling at all levels

- Function-level and line-level hotspot analysis, down to disassembly
- Call stack analysis
- Low overhead
- Mixed-language, multi-threaded application analysis
- Advanced hardware event analysis for native codes (Cython, C++, Fortran) for cache misses, branch misprediction, etc.

Feature	cProfile	Line_profiler	Intel® VTune™ Amplifier
Profiling technology	Event	Instrumentation	Sampling, hardware events
Analysis granularity	Function-level	Line-level	Line-level, call stack, time windows, hardware events
Intrusiveness	Medium (1.3-5x)	High (4-10x)	Low (1.05-1.3x)
Mixed language programs	Python	Python	Python, Cython, C++, Fortran

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Scaling Python with JIT Compilation

Stanley Seibert
Director of Community Innovation
Continuum Analytics
November 2016

ANACONDA
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Creating a Compiler For Python

Many valid approaches, but we think these are the most important for data science:

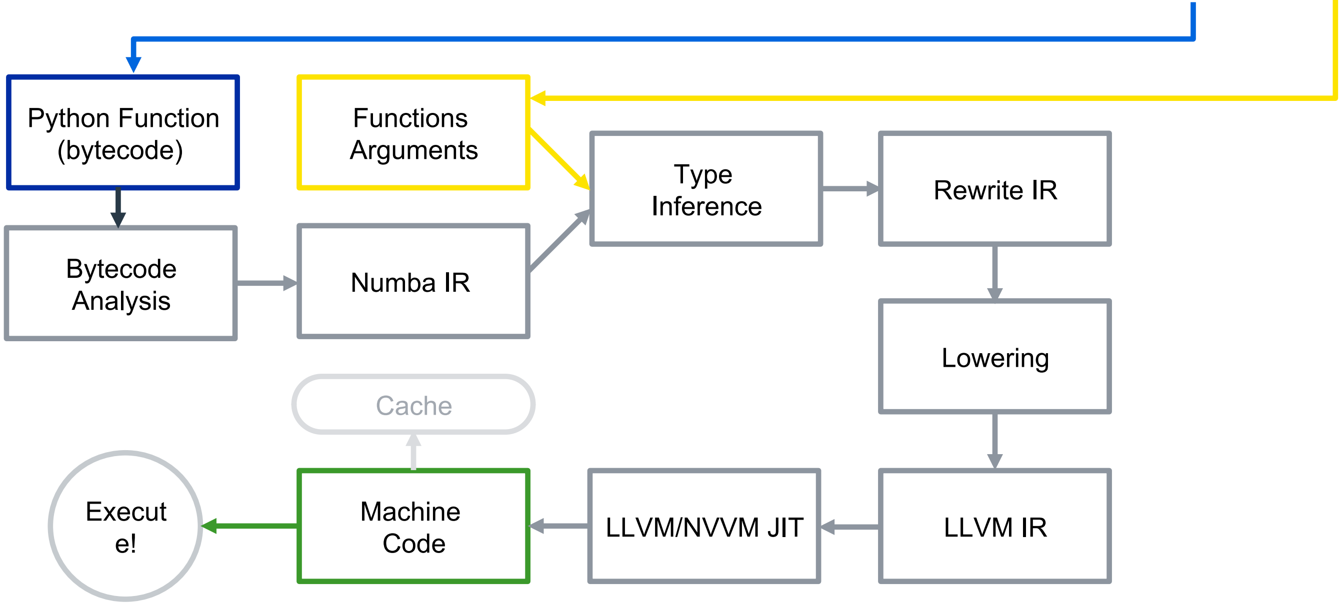
- **Cannot replace the standard interpreter**
  - Must be able to continue to use pandas, SciPy, scikit-learn, etc
- **Minimize boilerplate**
  - Traditional compiled Python extensions require a lot of infrastructure. Try to stay simple and get out of the way.
- **Be flexible about execution model**
  - Not all hardware is a general purpose CPU
- **Integrate well with Python's adaptable ecosystem**
  - Must be able to continue to use pandas, SciPy, scikit-learn, etc

Numba: A JIT Compiler for Python Functions

- An open-source, function-at-a-time compiler library for Python
- Compiler toolbox for different targets and execution models:
  - single-threaded CPU, multi-threaded CPU, GPU
  - regular functions, "universal functions" (array functions), GPU kernels
- Speedup: 2x (compared to basic NumPy code) to 200x (compared to pure Python)
- Combine ease of writing Python with speeds approaching FORTRAN
- Empowers data scientists who make tools for *themselves and other data scientists*

How does Numba work?

```
@jit
def do_math(a, b):
    …
>>> do_math(x, y)
```



Supported Platforms and Hardware

OS	HW	SW
Windows (7 and later)	32 and 64-bit x86 CPUs	Python 2 and 3
OS X (10.9 and later)	CUDA & HSA Capable GPUs	NumPy 1.7 through 1.11
Linux (RHEL 5 and later)	Experimental support for ARM, Xeon Phi, AMD Fiji GPUs	

Basic Example

In [87]:
```
@jit(nopython=True)
def nan_compact(x):
    out = np.empty_like(x)
    out_index = 0
    for element in x:
        if not np.isnan(element):
            out[out_index] = element
            out_index += 1
    return out[:out_index]
```

In [88]:
```
a = np.random.uniform(size=10000)
a[a < 0.2] = np.nan
np.testing.assert_equal(nan_compact(a), a[~np.isnan(a)])
```

In [89]:
```
%timeit a[~np.isnan(a)]
%timeit nan_compact(a)
```

```
10000 loops, best of 3: 52 µs per loop
100000 loops, best of 3: 19.6 µs per loop
```

Basic Example

Numba decorator (nopython=True not required)

Array Allocation

Looping over ndarray x as an iterator

Using numpy math functions

Returning a slice of the array

In [87]:
```
@jit(nopython=True)
def nan_compact(x):
    out = np.empty_like(x)
    out_index = 0
    for element in x:
        if not np.isnan(element):
            out[out_index] = element
            out_index += 1
    return out[:out_index]
```

In [88]:
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%timeit a[~np.isnan(a)]
%timeit nan_compact(a)
```

```
10000 loops, best of 3: 52 µs per loop
100000 loops, best of 3: 19.6 µs per loop
```

2.7x speedup!

Releasing the GIL

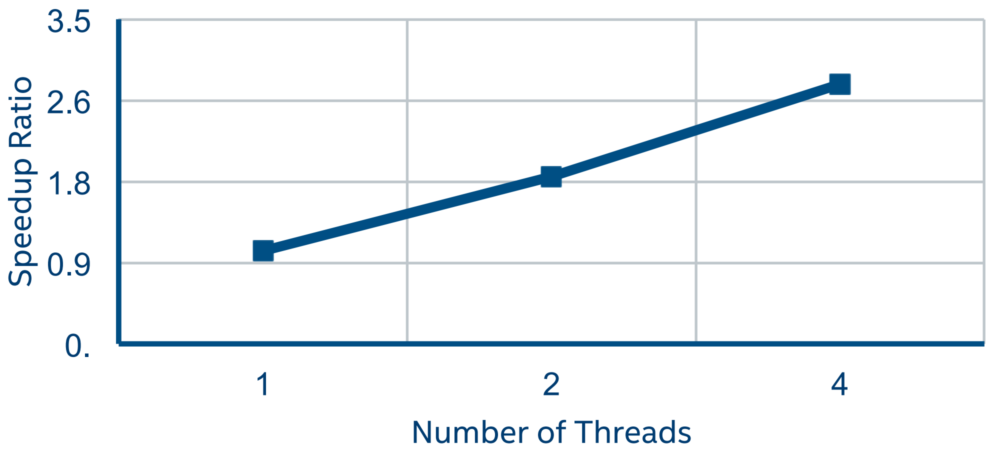
Option to release the GIL

```
In [14]: SQRT_2PI = np.sqrt(2 * np.pi)
         @numba.jit(nogil=True)
         def gaussian(x, mu, sigma):
             return np.exp(0.5 * ((x - mu)**2) / sigma) / (sigma * SQRT_2PI)

         print(gaussian(0.5, 1.5, 1.0))

0.657744623479
```

Using Python concurrent.futures



Universal Functions (Ufuncs)

Ufuncs are a core concept in NumPy for array-oriented computing.

- A function with scalar inputs is broadcast across the elements of the input arrays:
  - np.add([1,2,3], 3) == [4, 5, 6]
  - np.add([1,2,3], [10, 20, 30]) == [11, 22, 33]
- Parallelism is present, by construction. Numba will generate loops and can automatically multi-thread if requested.
- Before Numba, creating fast ufuncs required writing C. No longer!

Universal Functions (Ufuncs)

In [13]:

```
@numba.vectorize
def response(v, gamma):
    if v < 0:
        return 0.0
    elif v < 1:
        return v ** gamma
    else:
        return v
```

Different decorator!

In [14]:

```
x = np.linspace(-1, 2, 10000)
gamma = 1.7
%timeit np.piecewise(x, [x < 0, x >= 1],[0.0, lambda x: x, lambda x: x**gamma])
%timeit response(x, gamma)
```

```
1000 loops, best of 3: 244 µs per loop
The slowest run took 411.51 times longer than the fastest. This could mean that an intermedia
te result is being cached.
10000 loops, best of 3: 136 µs per loop
```

1.8x speedup!

Multi-threaded Ufuncs

Specify type signature

```
In [12]: SQRT_2 = np.sqrt(2)

         @numba.vectorize('float64(float64, float64, float64)', target='parallel')
         def gaussian_cdf_parallel(x, mu, sigma):
             return 0.5 * (1 + math.erf( (x - mu) / (sigma * SQRT_2)))
```

Select parallel target

Automatically uses all CPU cores!

Distributed Computing Example: Dask

Dask Client (Haswell)

Dask Scheduler

f(x)

Dask Worker (Skylake)

f(x)

Dask Worker (Skylake)

f(x)

Dask Worker (Knight's Landing)

```
@jit
def f(x):
    ...
```

- Serialize with pickle module
- Works with Dask and Spark (and others)
- Automatic recompilation for each target

DASK

Other Numba Features

- Detects CPU model during code generation and instructs LLVM to optimize for that architecture.
- Automatic dispatch to multiple type-specialized implementations of the same function
- Uses LLVM autovectorization optimization passes for SIMD code generation
- Supports calls directly to C with CFFI and ctypes
- Optional caching of compiled functions to disk
- Ahead of time compilation to shared libraries
- Extension API allowing 3rd parties to extend the compiler with new data types and functions.

Conclusion

- Numba - Create new high performance functions on-the-fly with pure Python
- Understands NumPy arrays and many NumPy operations
- Supplies several compilation modes and options for multi-threading
- Use with your favorite distributed computing framework

- For more information: http://numba.pydata.org
- Comes with Anaconda: https://www.continuum.io/downloads

Numba

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Call To Action

Intel is working with community leaders like Continuum Analytics to bring the BEST performance on IA to Python developers

- Start with either Intel’s or Continuum’s distribution
  - Both have Intel performance goodness baked in!
  - You cannot go wrong either way!
- Give Numba* a try and see performance increase
- Try Python* performance profiling with Intel® VTune™ Amplifier!

- Intel Distribution for Python is free!

  `https://software.intel.com/en-us/intel-distribution-for-python`

  – Commercial support included for Intel® Parallel Studio XE customers!

  – Easy to install with Anaconda* `https://anaconda.org/intel/`

Thank you for your time

Stan Seibert

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www.intel.com/hpcdevcon

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