CONTINUUM ANALYTICS

Scaling PyData Up and Out

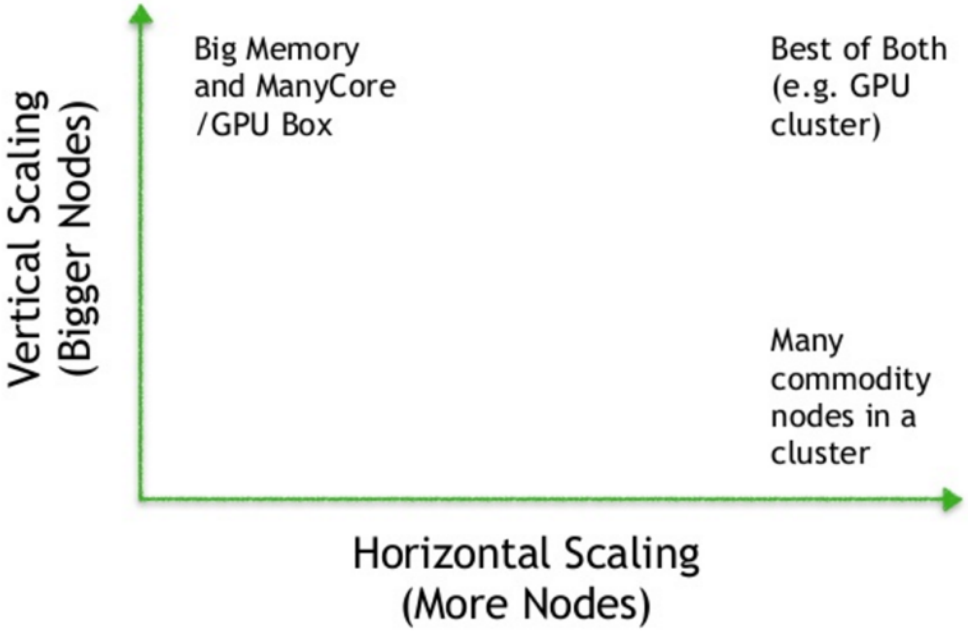
Making NumPy- and Pandas-style code faster and run in-parallel.

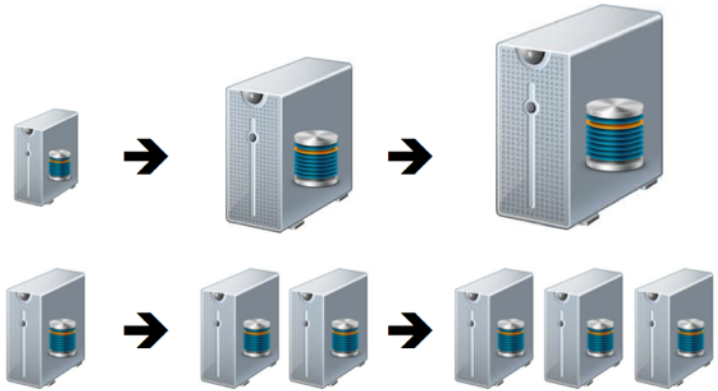
Travis E. Oliphant, PhD

Python Enthusiast since 1997

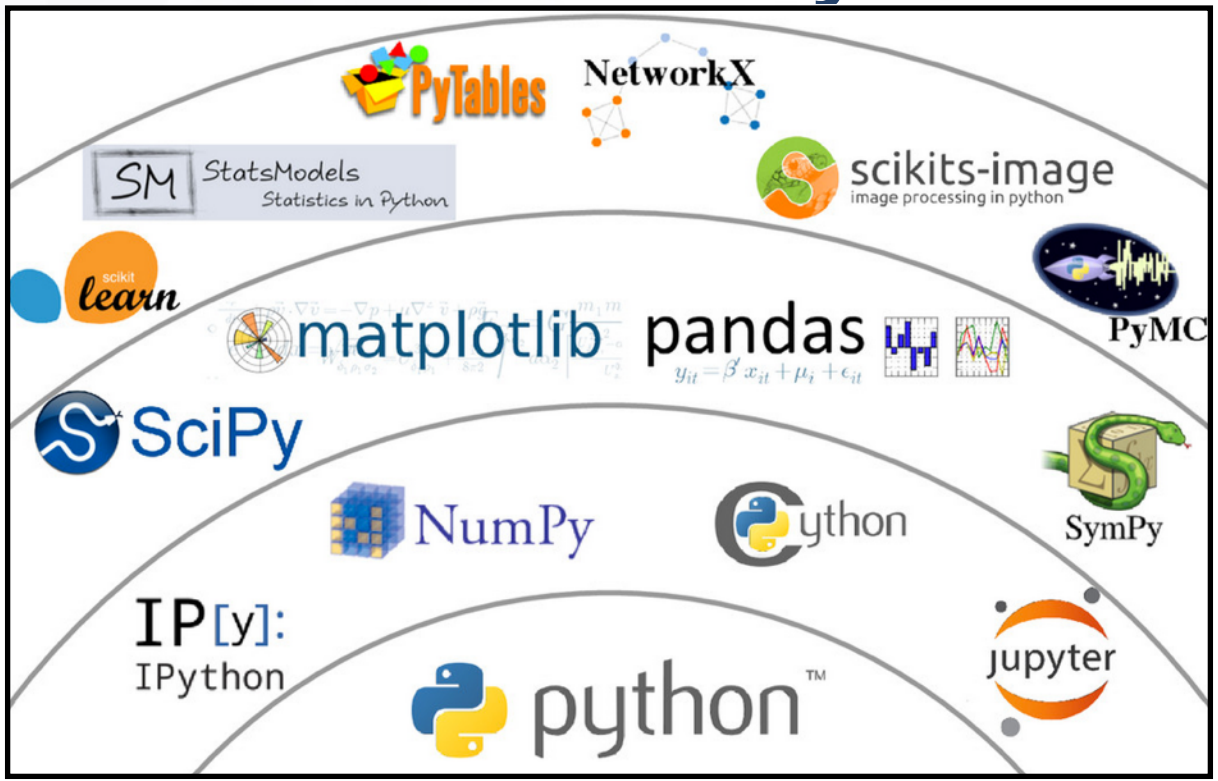
ANACONDA

Scaling Up vs. Out





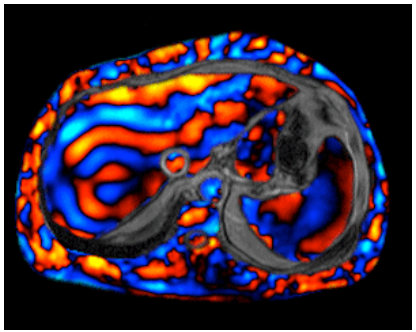
"Python's Scientific Ecosystem"



@jakevdp

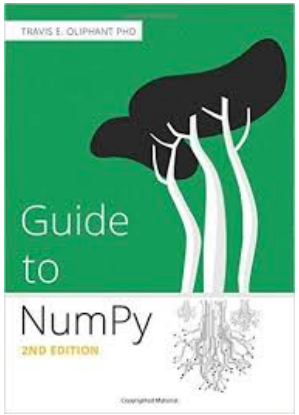
ANACONDA

I spent the first 15 years of my "Python life" working to build the foundation of the Python Scientific Ecosystem as a practitioner/developer



SciPy

NumPy



python

PEP 357
PEP 3118

I plan to spend the next 15 years ensuring this ecosystem can scale both up **and** out as an entrepreneur, evangelist, and innovator.

NUMFOCUS
OPEN CODE = BETTER SCIENCE

PyData

ANACONDA
Powered by Continuum Analytics

CONDA
NUMBA
DASK
DYND
BLAZE
DATA-FABRIC

ANACONDA

In 2012 we “took off” in this effort to form the foundation of scalable Python — Numba (scale-up) and Blaze (scale-out) were the major efforts.

In early 2013, I “retired” from NumPy maintenance to pursue “next-generation” NumPy.

Not so much a single new library, but a new emphasis

Rally a community

NUMFOCUS
OPEN CODE = BETTER SCIENCE

"Apache" for Open Data Science

PyData

Community-led Conference Series with sponsorship proceeds going directly to NumFocus

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Organize a company

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Purpose

Empower people to solve the world's greatest challenges.

Mission

We help people discover, analyze, and collaborate by connecting their curiosity and experience with any data.

Start working on key technology

Blaze — blaze, odo, datashape, dynd, **dask**
Bokeh — interactive visualization
Numba — Array-oriented Python subset compiler

Conda — Cross-platform package manager
with environments

Bootstrap (self) and seed funding through 2014
VC funded in 2015

Milestone success — 2016

Numba is delivering on scaling out

- NumPy's ufuncs on multiple CPU and GPU threads
- General GPU code
- General CPU code

Dask is delivering on scaling up

- **dask.array** (numpy scaled up)
- **dask.dataframe** (pandas scaled up)
- **dask.bag** (lists scaled up)
- **dask.delayed** (general scale-up construction)

Numba + Dask

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Look at **all** of the data with **Bokeh's datashader.**
Decouple the data-processing from the visualization.
Visualize arbitrarily large data.

E.g. Open Street Map data:

- About **3 billion** GPS coordinates
- https://blog.openstreetmap.org/2012/04/01/bulk-gps-point-data/.
- This image was rendered in one minute on a standard MacBook with 16 GB RAM
- Renders in a milliseconds on several 128GB Amazon EC2 instances

Categorical data: 2010 US Census

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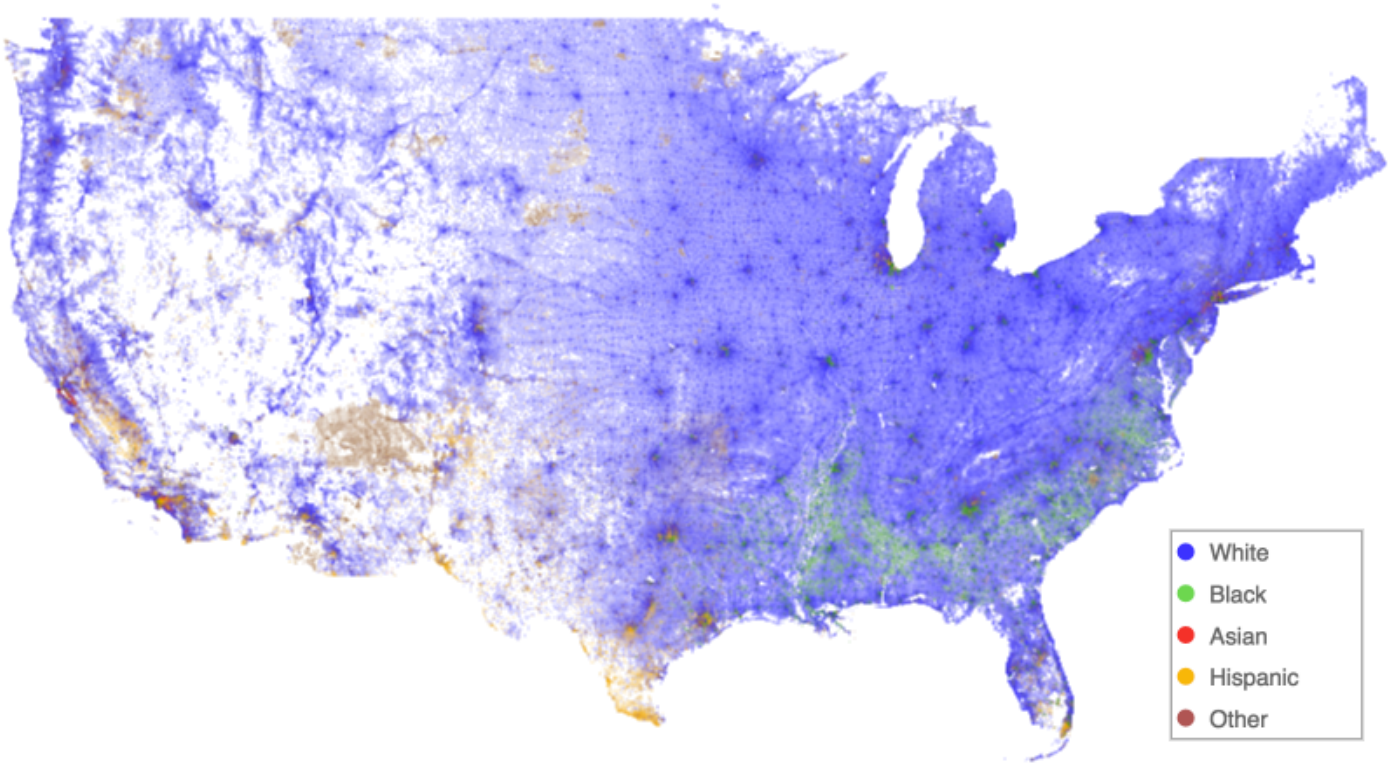

- One point per person
- 300 million total
- Categorized by race
- Interactive rendering with Numba+Dask
- No pre-tiling

Easiest way to get everything!

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ANACONDA® is….

the Leading Open Data Science Platform
powered by Python…
the fastest growing open data science language

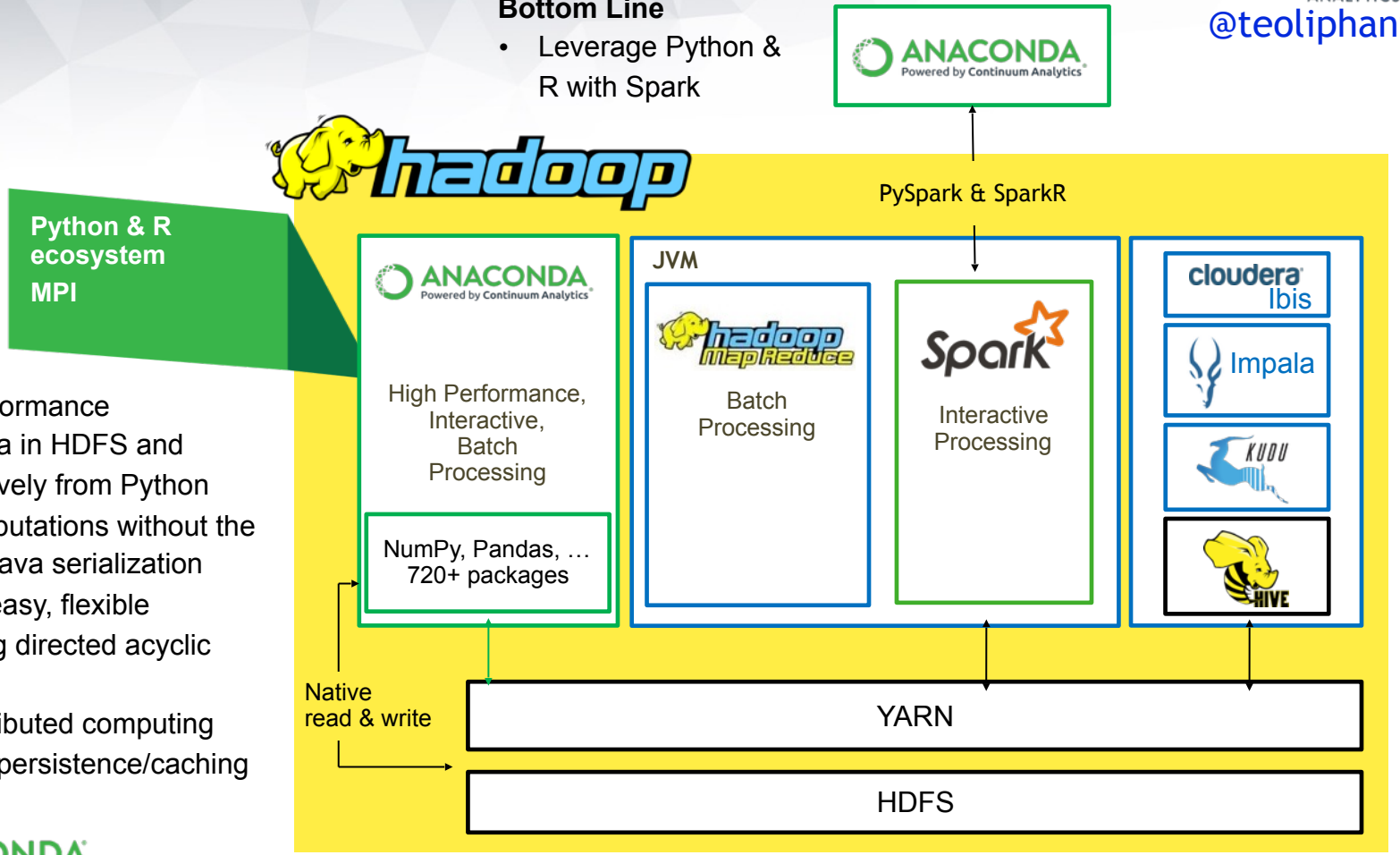
- **Accelerate Time-to-Value**
- **Connect Data, Analytics & Compute**
- **Empower Data Science Teams**

Anaconda now with MKL as default

- Intel MKL (Math Kernel Libraries) provide enhanced algorithms for basic math functions.
- Using MKL provides optimal performance for basic BLAS, LAPACK, FFT, and math functions.
- Anaconda since version 2.5 has MKL provided as the default in the free download of Anaconda (you can also distribute binaries linked against these MKL-enhanced tools).

Bottom Line

- Leverage Python & R with Spark



Bottom Line

10-100X faster performance

- Interact with data in HDFS and Amazon S3 natively from Python
- Distributed computations without the JVM & Python/Java serialization
- Framework for easy, flexible parallelism using directed acyclic graphs (DAGs)
- Interactive, distributed computing with in-memory persistence/caching

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Overview of Numba

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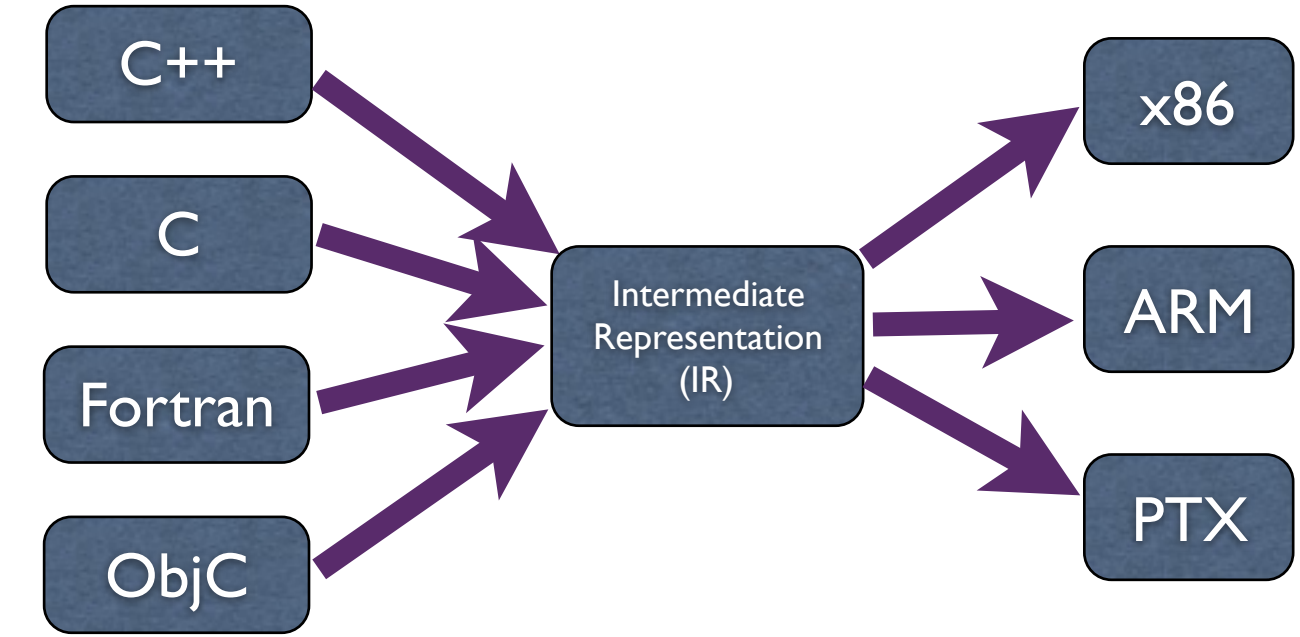
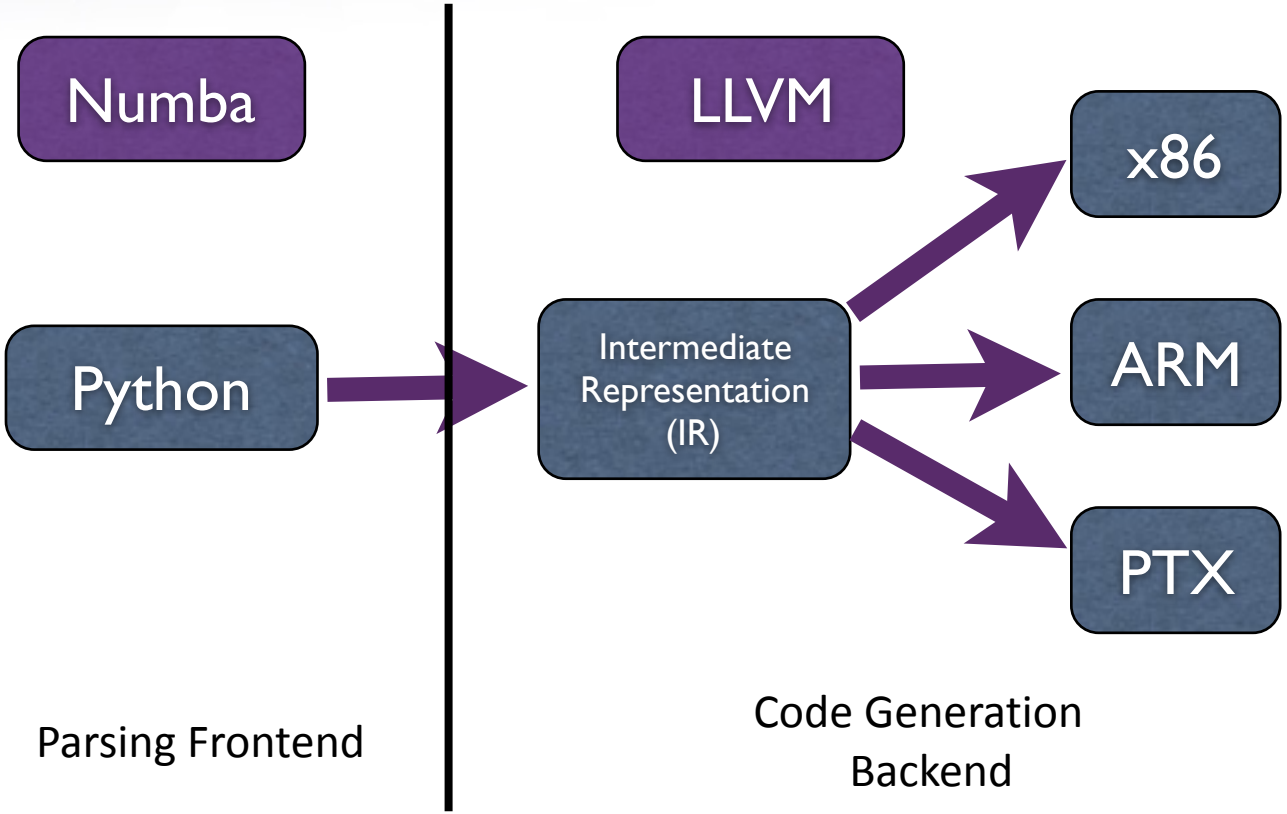
Compiler overview

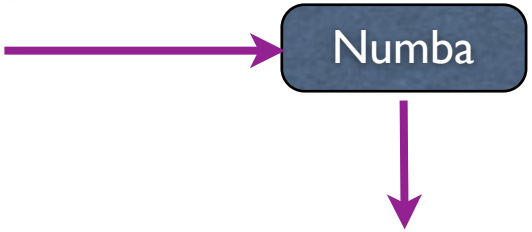


Compiler overview



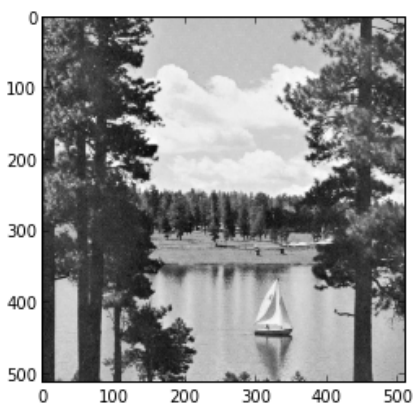
Example

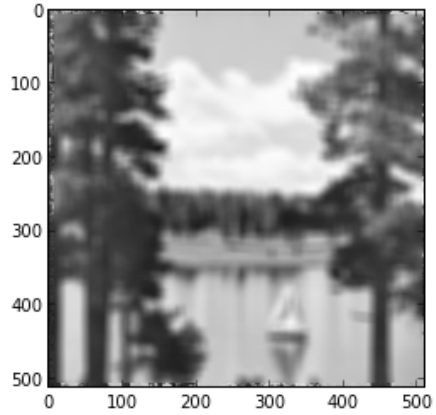

```python
@numba.jit
def simple():
    total = 0.0
    for i in range(9999):
        for j in range(1,9999):
            total += (i / j)
    return total
```




```
define double @__numba_specialized_0___main___2E_simple() nounwind readnone {
entry:
  br label %"for_condition_7:17.preheader"

"for_condition_7:17.preheader":                   ; preds = %"exit_for_7:8", %entry
  %total_28 = phi double [ 0.000000e+00, %entry ], [ %3, %"exit_for_7:8" ]
  %storemerge7 = phi i64 [ 0, %entry ], [ %0, %"exit_for_7:8" ]
  br label %"loop_body_8:12"

"exit_for_6:4":                                   ; preds = %"exit_for_7:8"
  ret double %3

"exit_for_7:8":                                   ; preds = %"loop_body_8:12"
  %0 = add i64 %storemerge7, 1
  %exitcond9 = icmp eq i64 %0, 9999
  br i1 %exitcond9, label %"exit_for_6:4", label %"for_condition_7:17.preheader"

"loop_body_8:12":                                 ; preds = %"loop_body_8:12", %"for_condition_7:17.prel
  %lsr.iv = phi i64 [ %lsr.iv.next, %"loop_body_8:12" ], [ 1, %"for_condition_7:17.preheader" ]
  %total_36 = phi double [ %total_28, %"for_condition_7:17.preheader" ], [ %3, %"loop_body_8:12" ]
  %1 = sdiv i64 %storemerge7, %lsr.iv
  %2 = sitofp i64 %1 to double
  %3 = fadd double %total_36, %2
  %lsr.iv.next = add i64 %lsr.iv, 1
  %exitcond = icmp eq i64 %lsr.iv.next, 9999
  br i1 %exitcond, label %"exit_for_7:8", label %"loop_body_8:12"
}
```

Image Processing



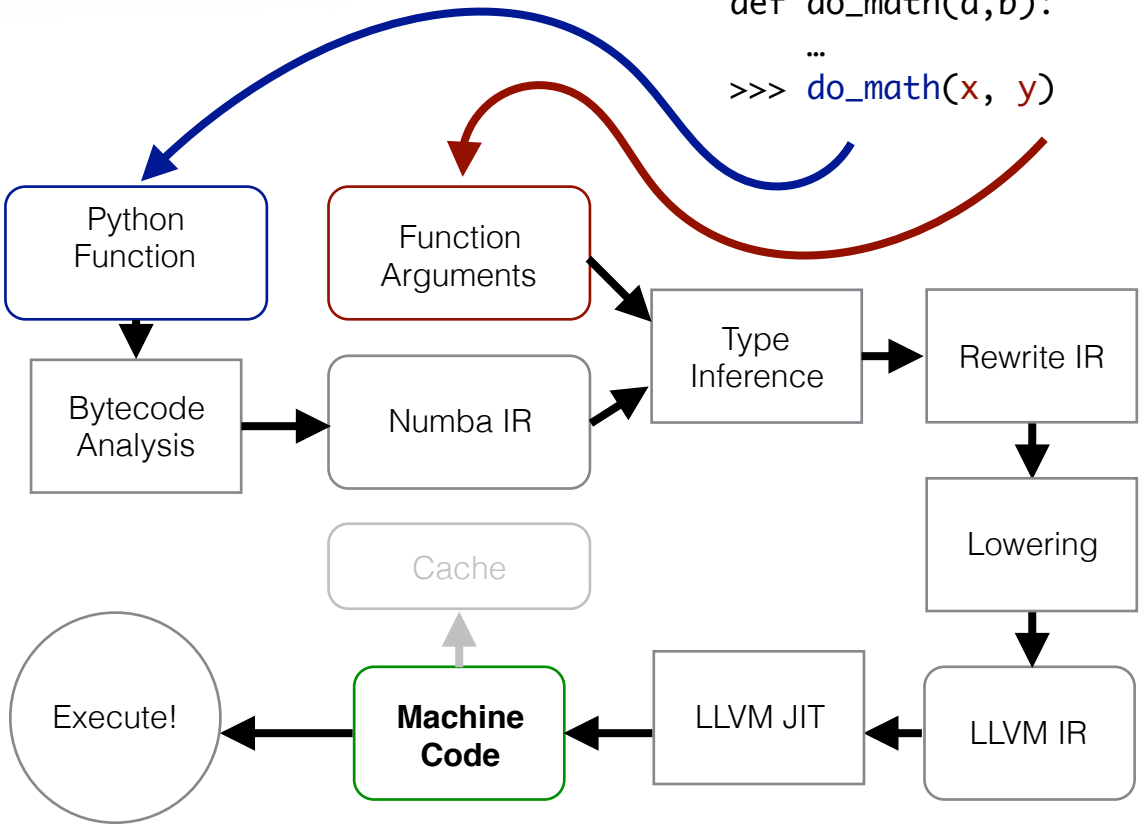


~1500x speed-up

```
@jit('void(f8[:,:],f8[:,:],f8[:,:])')
def filter(image, filt, output):
    M, N = image.shape
    m, n = filt.shape
    for i in range(m//2, M-m//2):
        for j in range(n//2, N-n//2):
            result = 0.0
            for k in range(m):
                for l in range(n):
                    result += image[i+k-m//2,j+l-n//2]*filt[k, l]
            output[i,j] = result
```

How Numba works


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



Numba Features

- Numba supports:
  - Windows, OS X, and Linux
  - 32 and 64-bit x86 CPUs and NVIDIA GPUs
  - Python 2 and 3
  - NumPy versions 1.6 through 1.9
- Does *not* require a C/C++ compiler on the user's system.
- < 70 MB to install.
- Does *not* replace the standard Python interpreter
  (all of your existing Python libraries are still available)

Numba Modes

- *object mode:* Compiled code operates on Python objects. Only significant performance improvement is compilation of loops that can be compiled in nopython mode (see below).

- *nopython mode:* Compiled code operates on "machine native" data. Usually within 25% of the performance of equivalent C or FORTRAN.

How to Use Numba

1. Create a realistic benchmark test case.
   (Do not use your unit tests as a benchmark!)
2. Run a profiler on your benchmark.
   (cProfile is a good choice)
3. Identify hotspots that could potentially be compiled by Numba with a little refactoring.
   (see rest of this talk and online documentation)
4. Apply @numba.jit and @numba.vectorize as needed to critical functions.
   (Small rewrites may be needed to work around Numba limitations.)
5. Re-run benchmark to check if there was a performance improvement.

The Basics

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
```

The Basics

Numba decorator (nopython=True not required)

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]
```

Array Allocation

Looping over ndarray x as an iterator

Using numpy math functions

Returning a slice of the array

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 over NumPy!

Calling Other Functions

In [85]:
```
@jit
def norm(vec):
    mag = 0.0
    for element in vec:
        mag += element**2
    mag **= 0.5

    ret = np.empty_like(vec)
    for i, element in enumerate(vec):
        ret[i] = element / mag

    return ret

@jit
def clamp(x):
    if x > 1.0:
        return 1.0
    elif x < -1.0:
        return -1.0
    else:
        return x

@jit
def angle_between(vec1, vec2):
    norm_vec1 = norm(vec1)
    norm_vec2 = norm(vec2)

    cos_angle = (norm_vec1 * norm_vec2).sum()
    return np.arccos(clamp(cos_angle))
```

Calling Other Functions

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    norm_vec1 = norm(vec1)
    norm_vec2 = norm(vec2)

    cos_angle = (norm_vec1 * norm_vec2).sum()
    return np.arccos(clamp(cos_angle))
```

This function is not inlined

This function is inlined

9.8x speedup compared to doing this with numpy functions

NumPy Ufuncs

NumPy ufuncs (and gufuncs) are functions that operate “element-wise” (or “sub-dimension-wise”) across an array without an explicit loop.

This implicit loop (which is in machine code) is at the core of why NumPy is fast. Dispatch is done internally to a particular code-segment based on the type of the array. It is a very powerful abstraction in the scientific computing stack.

Making new ufuncs used to be only possible in C — painful!

Making Ufuncs with Numba

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In [7]:
```
@numba.vectorize(nopython=True)
def game_wins(win_probability, max_wins, max_losses):
    wins = 0
    losses = 0
    while wins < max_wins and losses < max_losses:
        if np.random.rand() < win_probability:
            wins += 1
        else:
            losses += 1

    return wins
```

In [21]:
```
sim_input = np.tile(np.linspace(0.0, 1.0, 100), (5000, 1))
sim_results = game_wins(sim_input, 12, 3)
```

In [22]:
```
%timeit game_wins(sim_input, 12, 3)
```

```
10 loops, best of 3: 50 ms per loop
```

Case-study -- j0 from scipy.special

- scipy.special was one of the first libraries I wrote (in 1999)
- extended Numeric's umath module by adding new universal functions (ufuncs) to compute many scientific functions by wrapping C and Fortran libs.

- Bessel functions are solutions to a particular differential equation:

$$x^2 \frac{d^2y}{dx^2} + x\frac{dy}{dx} + (x^2 - \alpha^2)y = 0$$

$$y = J_\alpha(x)$$

$$J_n(x) = \frac{1}{\pi}\int_0^\pi \cos(n\tau - x\sin(\tau))\, d\tau$$

scipy.special.j0 wraps cephes algorithm

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```
@jit('f8(f8)')
def j0(x):
    if (x < 0):
        x = -x

    if (x <= 5.0):
        z = x * x
        if (x < 1.0e-5):
            return (1.0 - z / 4.0)
        p = (z-DR1) * (z-DR2)
        p = p * polevl(z, RP) / polevl(z, RQ)
        return p

    w = 5.0 / x
    q = 25.0 / (x*x)
    p = polevl(q, PP) / polevl(q, PQ)
    q = polevl(q, QP) / p1evl(q, QQ)
    xn = x - NPY_PI_4
    p = p*math.cos(xn) - w * q * math.sin(xn)
    return p * SQ2OPI / math.sqrt(x)

vj0 = vectorize(['f8(f8)'])(j0)
```

Don’t need this anymore!

```
@jit('f8(f8,f8[:])')
def polevl(x, coef):
    N = len(coef)
    ans = coef[0]
    i = 1
    while i < N:
        ans = ans * x + coef[i]
        i += 1
    return ans

@jit('f8(f8,f8[:])')
def p1evl(x, coef):
    N = len(coef)
    ans = x + coef[0]
    i = 1
    while i < N:
        ans = ans * x + coef[i]
        i += 1
    return ans
```

```
DR1 = 5.783185962946784521175995758455807035071
DR2 = 30.471262343662086399078163175022755848 42

NPY_PI_4 = .7853981633974483096
SQ2OPI   = .797884560802865355879 89
```

```
QP = np.array([
-1.1366383889846914 9931E-2,
-1.2825271867050931 8512E0,
-1.9553954425773597 2385E1,
-9.3206015212376823 1369E1,
-1.7768116798048805 0595E2,
-1.4707750515495117 0175E2,
-5.1410532676659933 0220E1,
-6.0501435060072848 1186E0], 'd')

QQ = np.array([
   # 1.0000000000000000000E0,
  6.4317825611817802 3184E1,
  8.5643002597698058 7198E2,
  3.8824018360540160 9683E3,
  7.2404677419565247 8189E3,
  5.9307270118731698 4827E3,
  2.0620933166032784 7417E3,
  2.4200574024029139 3179E2], 'd')

PP = np.array([
  7.9693672929734705 1624E-4,
  8.2835239210744079 9803E-2,
  1.2395337164641429 9388E0,
  5.4472500305876875 090E0,
  8.7471650019981701 1941E0,
  5.3032403823539489 2183E0,
  9.9999999999999997 821E-1], 'd')

PQ = np.array([
  9.2440881055886363 7013E-4,
  8.5628847435447443 1428E-2,
  1.2535274390105895 3537E0,
  5.4709774033041710 5182E0,
  8.7619088323706959 4232E0,
  5.3060528823539461 7618E0,
  1.0000000000000000 218E0], 'd')
```

```
RP = np.array([
-4.7944322097820177 3821E9,
 1.9561749194655657 7543E12,
-2.4924834436096771 6204E14,
 9.7086225104730632 3952E15], 'd')

RQ = np.array([
    # 1.0000000000000000000E0,
 4.9956314715265101 7219E2,
 1.7378540167637468 3123E5,
 4.8440965833996204 5305E7,
 1.1185553704535683 4862E10,
 2.1127752011548921 7587E12,
 3.1051822985742258 3814E14,
 3.1812195594320494 3306E16,
 1.7108629408104313 6091E18], 'd')
```

Result --- equivalent to compiled code


```
In [6]: %timeit vj0(x)
10000 loops, best of 3: 75 us per loop

In [7]: from scipy.special import j0

In [8]: %timeit j0(x)
10000 loops, best of 3: 75.3 us per loop
```

But! Now code is in Python and can be experimented with more easily (and moved to the GPU / accelerator more easily)!

Numba is now popular!

A numba mailing list reports experiments of a SciPy author who got 2x speed-up by removing their Cython type annotations and surrounding function with numba.jit (with a few minor changes needed to the code).

With Numba's ahead-of-time compilation one can now legitimately use Numba to create a library that you ship to others (who then don't need to have Numba installed).

SciPy (and NumPy) would look very different in Numba had existed 16 years ago when SciPy was getting started — and the PyPy crowd would be happier.

Releasing the GIL

In [22]:
```
from concurrent.futures import ThreadPoolExecutor

@jit(nopython=True)
def mag2(z):
    return z.real * z.real + z.imag * z.imag

MAX_ITERS=250

@jit(nopython=True)
def mandel(c):
    z = 0j
    for i in range(MAX_ITERS):
        z = z*z + c
        if mag2(z) >= 4:
            return 255 * i // MAX_ITERS
    return 255

@jit(nogil=True, nopython=True)
def mandel_patch(args):
    rmin, rmax, nr, imin, imax, ni = args
    points = np.empty(nr*ni, dtype=np.complex128)
    values = np.empty(nr*ni, dtype=np.uint8)

    for i, c in enumerate(complex_grid(rmin, rmax, nr, imin, imax, ni)):
        points[i] = c
        values[i] = mandel(c)

    return points, values
```

Only nopython mode functions can release the GIL

Releasing the GIL


```
In [24]: %%timeit
         with ThreadPoolExecutor(max_workers=1) as executor:
             results = list(executor.map(mandel_patch, patches))

1 loops, best of 3: 470 ms per loop

In [25]: %%timeit
         with ThreadPoolExecutor(max_workers=4) as executor:
             results = list(executor.map(mandel_patch, patches))

10 loops, best of 3: 168 ms per loop
```

2.8x speedup with 4 cores

CUDA Python (in open-source Numba!)

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```
@cuda.jit
def array_scale(src, dst, scale):
    tid = cuda.threadIdx.x
    blkid = cuda.blockIdx.x
    blkdim = cuda.blockDim.x

    i = tid + blkid * blkdim

    if i >= n:
        return

    dst[i] = src[i] * scale

src = np.arange(N, dtype=np.float)
dst = np.empty_like(src)

threadsperblock = 32
blockspergrid = (src.size + (threadsperblock - 1)) // threadsperblock

array_scale[blockspergrid, threadsperblock](src, dst, 5.0)
```

CUDA Development using Python syntax for optimal performance!

10-20x faster than CPU

You have to understand CUDA at least a little — writing kernels that launch in parallel on the GPU

Classic Example

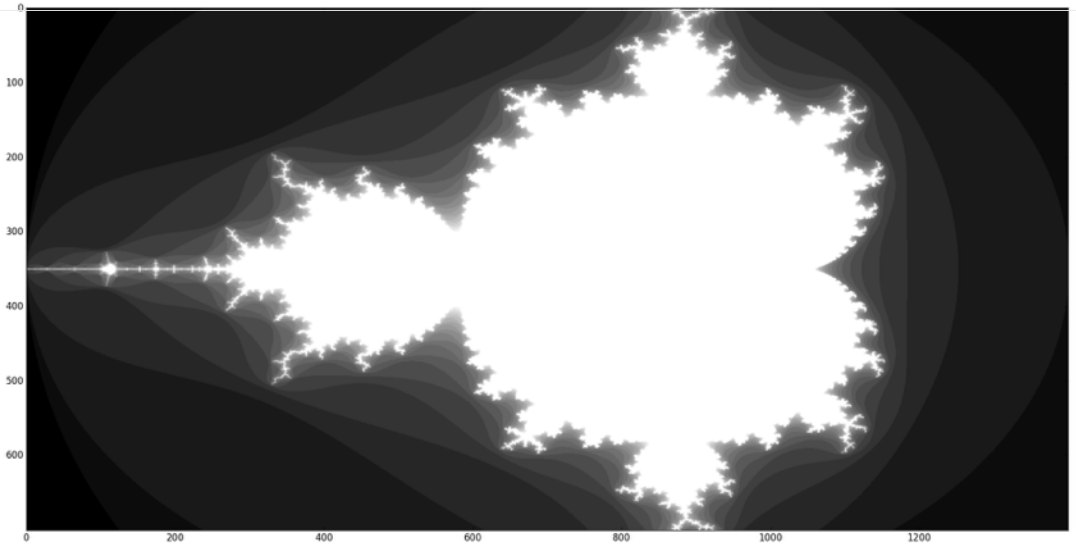
Mandelbrot

```
from numba import jit

@jit
def mandel(x, y, max_iters):
    c = complex(x,y)
    z = 0j
    for i in range(max_iters):
        z = z*z + c
        if z.real * z.real + z.imag * z.imag >= 4:
            return 255 * i // max_iters

    return 255
```

The Basics

Mandelbrot

CPython	1x
Numpy array-wide operations	13x
Numba (CPU)	120x
Numba (NVidia Tesla K20c)	2100x



Other interesting things

- CUDA Simulator to debug your code in Python interpreter
- Generalized ufuncs (@guvectorize) including GPU support and multi-core (threaded) support
- Call ctypes and cffi functions directly and pass them as arguments
- Support for types that understand the buffer protocol
- Pickle Numba functions to run on remote execution engines
- “numba annotate” to dump HTML annotated version of compiled code
- See: http://numba.pydata.org/numba-doc/0.23.0/

What Doesn't Work?

(A non-comprehensive list)

- lists, dictionaries, user defined classes (sets and tuples do work!)
- List and dictionary comprehensions
- Recursion
- Exceptions with non-constant parameters
- Most string operations (buffer support is very preliminary!)
- yield from
- closures inside a JIT function (compiling JIT functions inside a closure works…)
- Modifying globals
- Debugging of compiled code (you have to debug in Python mode).

Recently Added Numba Features

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- Support for named tuples in nopython mode
- Support for sets in nopython mode
- Limited support for lists in nopython mode
- On-disk caching of compiled functions (opt-in)
- JIT classes (zero-cost abstraction)
- Support of np.dot (and ‘@‘ operator on Python 3.5)
- Support for some of np.linalg
- generated_jit (jit the functions that are the return values of the decorated function)
- SmartArrays which can exist on host and GPU (transparent data access).
- Ahead of Time Compilation
- Disk-caching of pre-compiled code

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Overview of Dask as a Parallel Processing Framework with Distributed

ANACONDA®

Precursors to Parallelism

- Consider the following approaches first:
    1. Use better algorithms
    2. Try Numba or C/Cython
    3. Store data in efficient formats
    4. Subsample your data
- If you have to parallelize:
    1. Start with your laptop (4 cores, 16 GB RAM, 1 TB disk)
    2. Then a large workstation (24 cores, 1 TB RAM)
    3. Finally, scale out to a cluster

Overview of Dask

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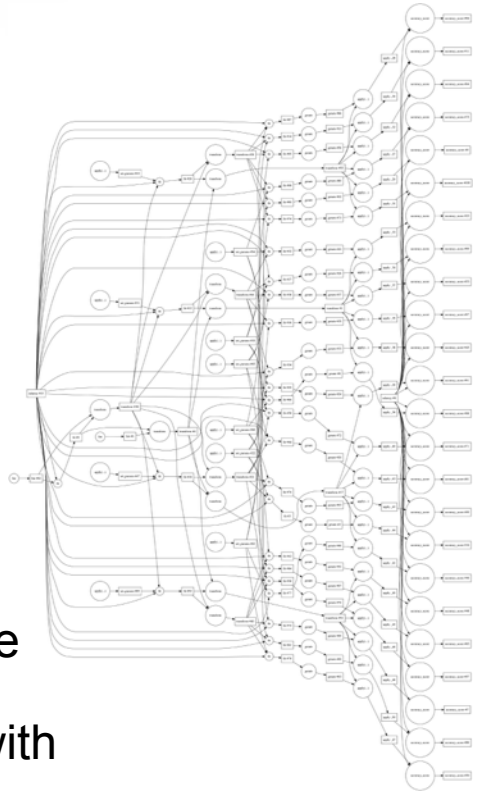
Dask is a Python parallel computing library that is:

- **Familiar**: Implements parallel NumPy and Pandas objects
- **Fast**: Optimized for demanding for numerical applications
- **Flexible**: for sophisticated and messy algorithms
- **Scales up**: Runs resiliently on clusters of 100s of machines
- **Scales down**: Pragmatic in a single process on a laptop
- **Interactive**: Responsive and fast for interactive data science



Dask **complements** the rest of Anaconda. It was developed with NumPy, Pandas, and scikit-learn developers.

Spectrum of Parallelization

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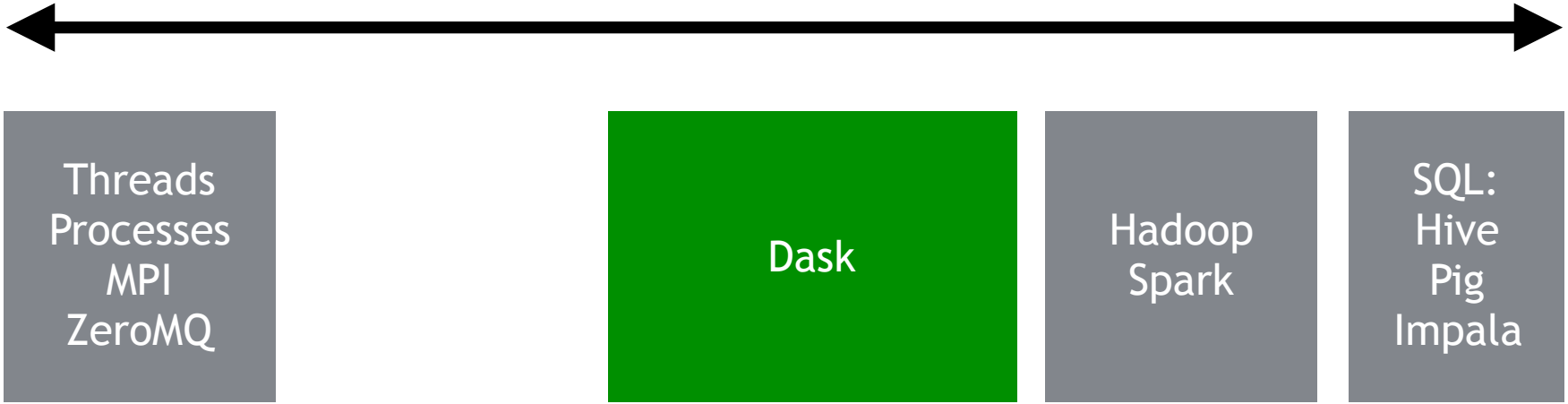
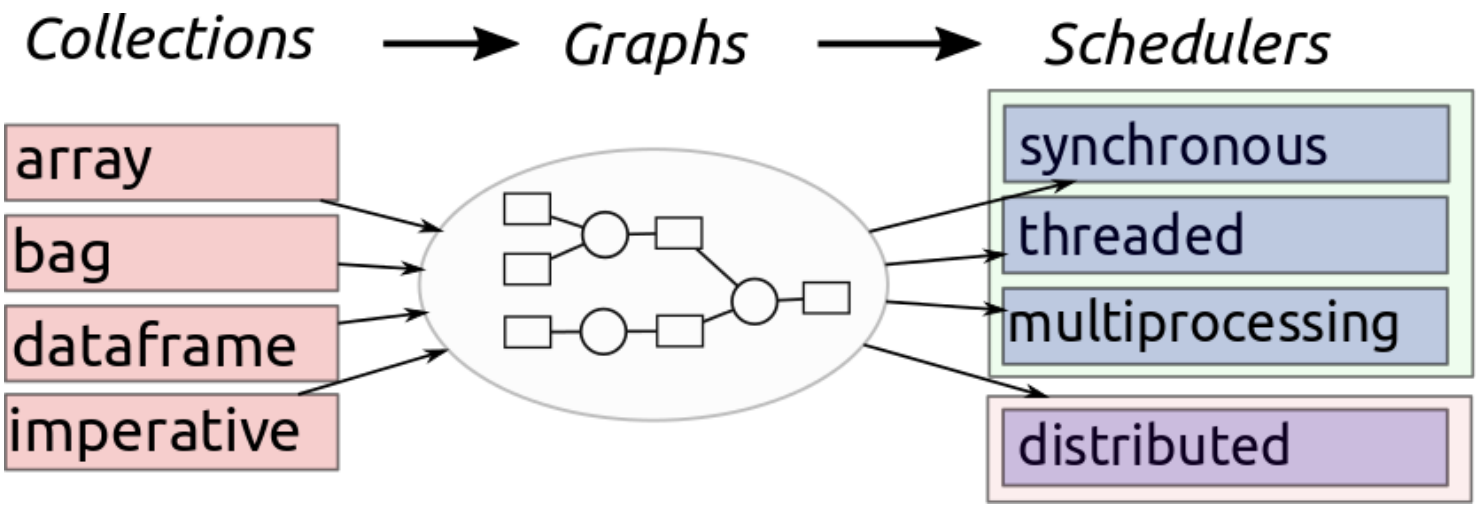
Explicit control: Fast but hard **Implicit control: Restrictive but easy**



Dask: From User Interaction to Execution



Dask Collections: Familiar Expressions and API

Dask array (mimics NumPy)

```
x.T - x.mean(axis=0)
```

Dask bag (collection of data)

```
b.map(json.loads).foldby(...)
```

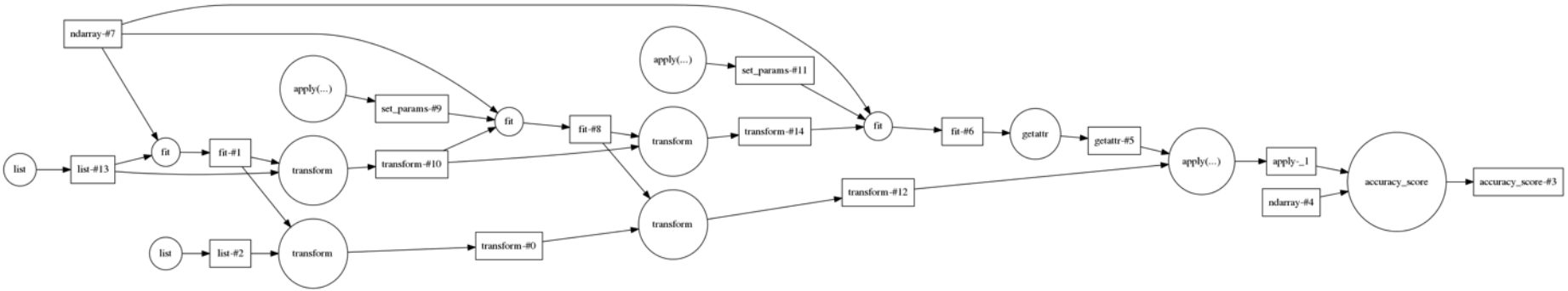
Dask dataframe (mimics Pandas)

```
df.groupby(df.index).value.mean()
```

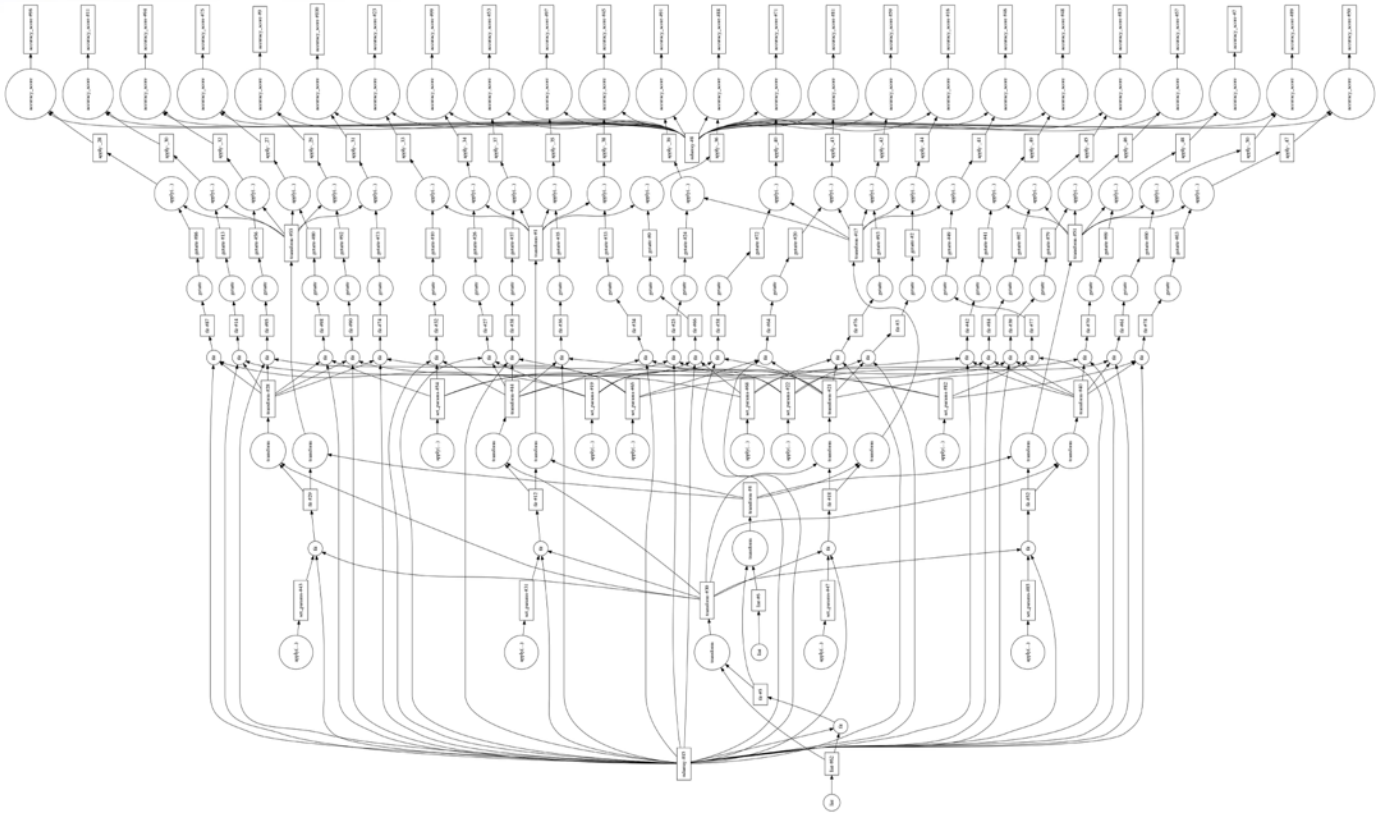
Dask imperative (wraps custom code)

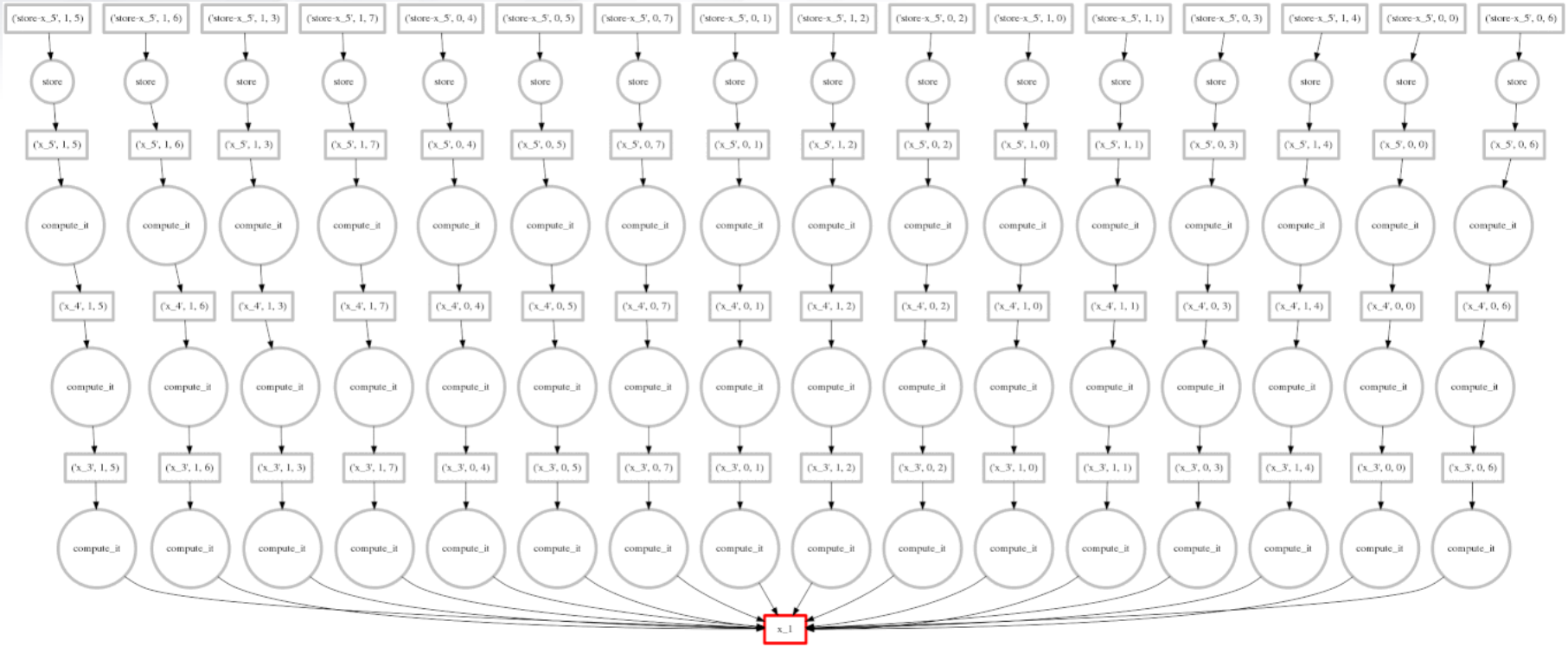
```
def load(filename):
def clean(data):
def analyze(result):
```

Dask Graphs: Example Machine Learning Pipeline



Dask Graphs: Example Machine Learning Pipeline + Grid Search

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compute_it
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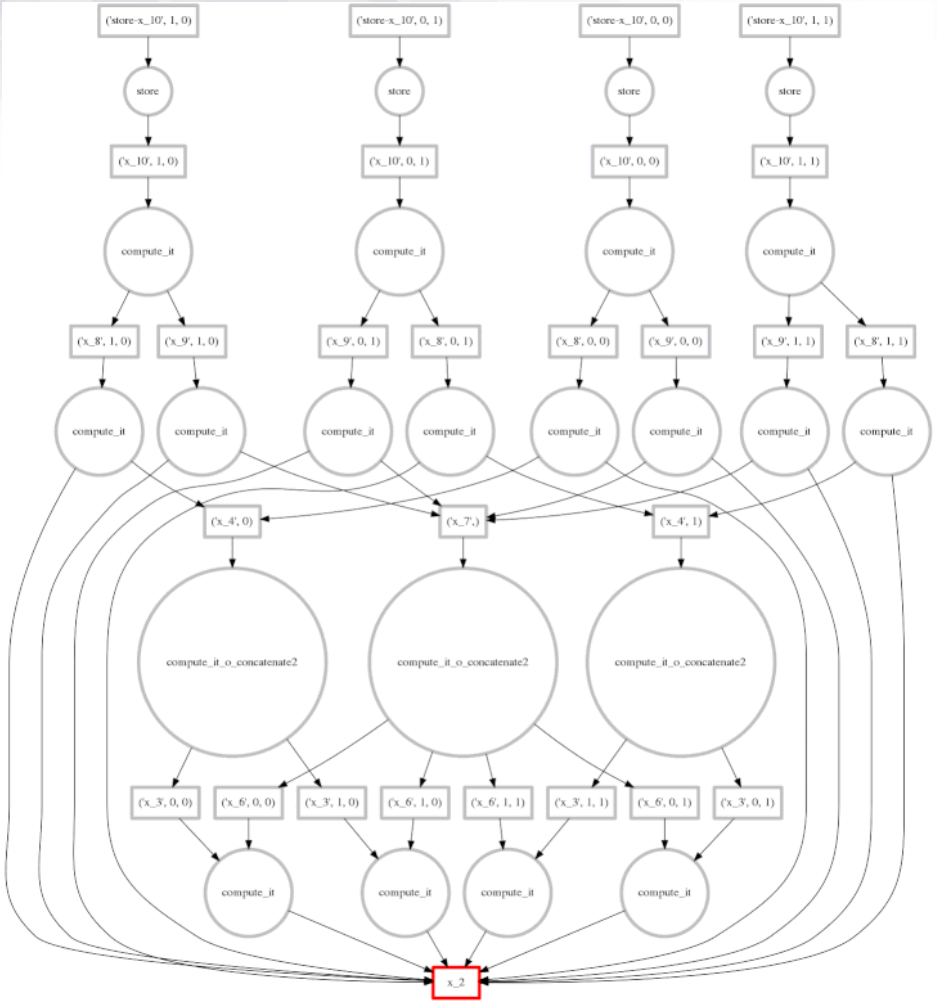
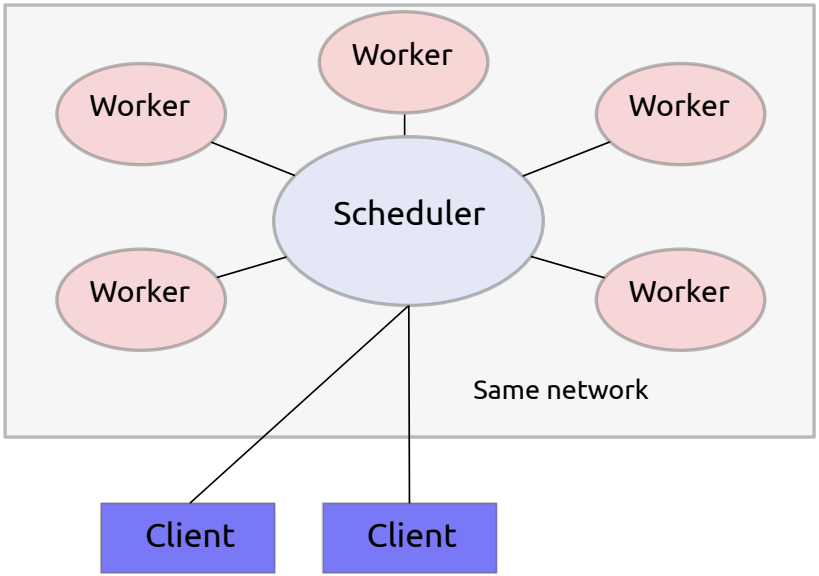
('x_3', 1, 1)
('x_3', 0, 3)
('x_3', 1, 4)
('x_3', 0, 0)
('x_3', 0, 6)
x_1

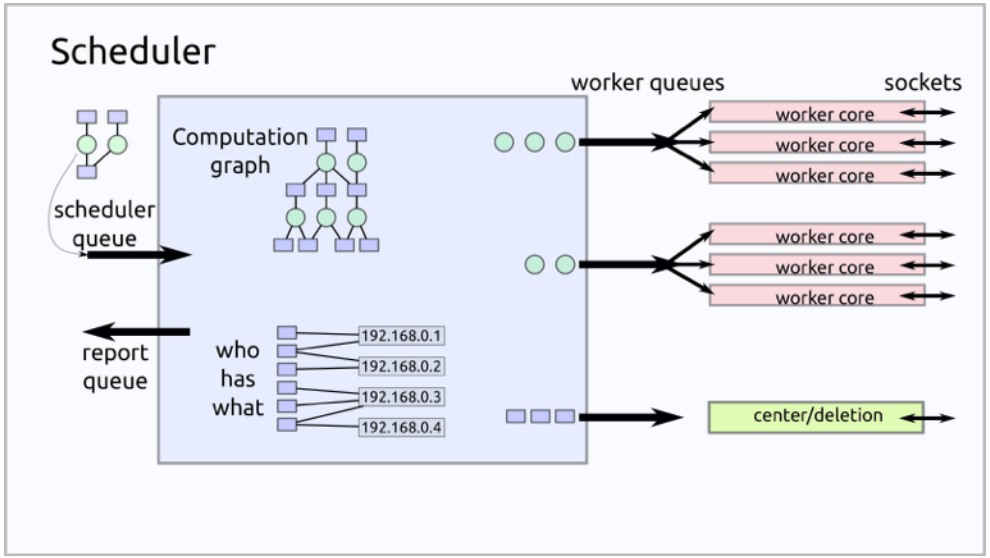
```
(((A + 1) * 2) ** 3)
```

```
(B - B.mean(axis=0))
+ (B.T / B.std())
```

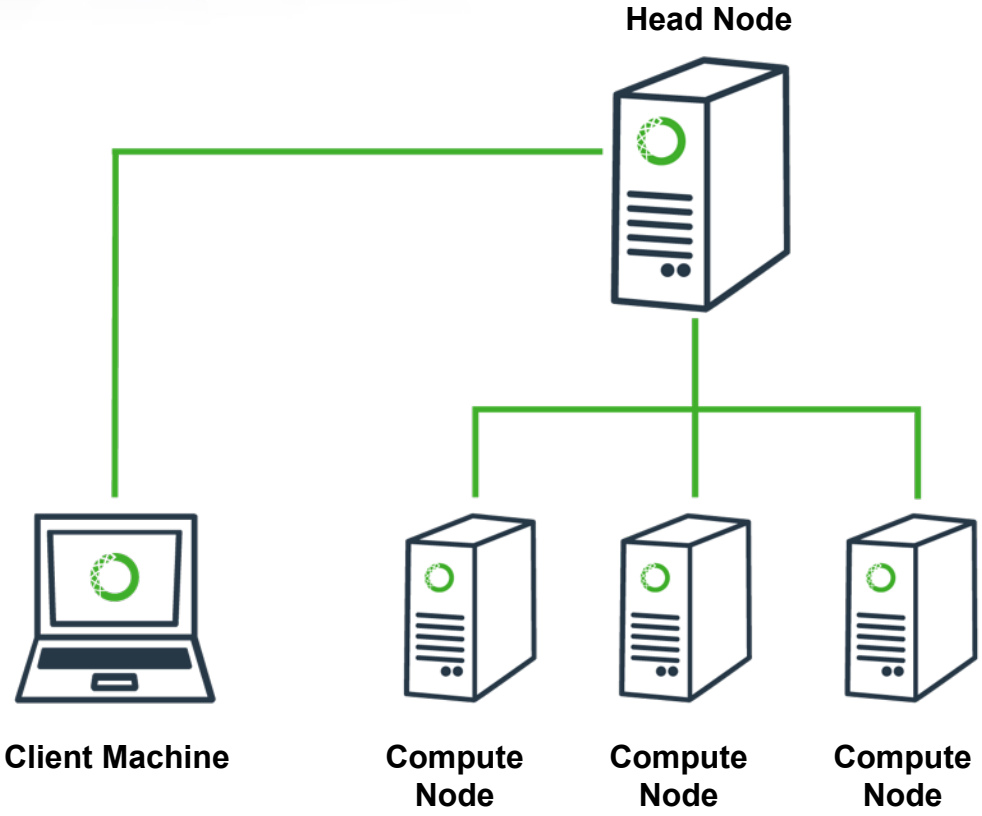


Dask Schedulers: Example - Distributed Scheduler





Cluster Architecture Diagram



Using Anaconda and Dask on your Cluster

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- Single machine with multiple threads or processes
- On a cluster with **SSH** (dcluster)
- Resource management: **YARN** (knit), **SGE**, **Slurm**
- On the cloud with **Amazon EC2** (dec2)
- On a cluster with **Anaconda for cluster management**
  - Manage multiple conda environments and packages on bare-metal or cloud-based clusters

Scheduler Visualization with Bokeh

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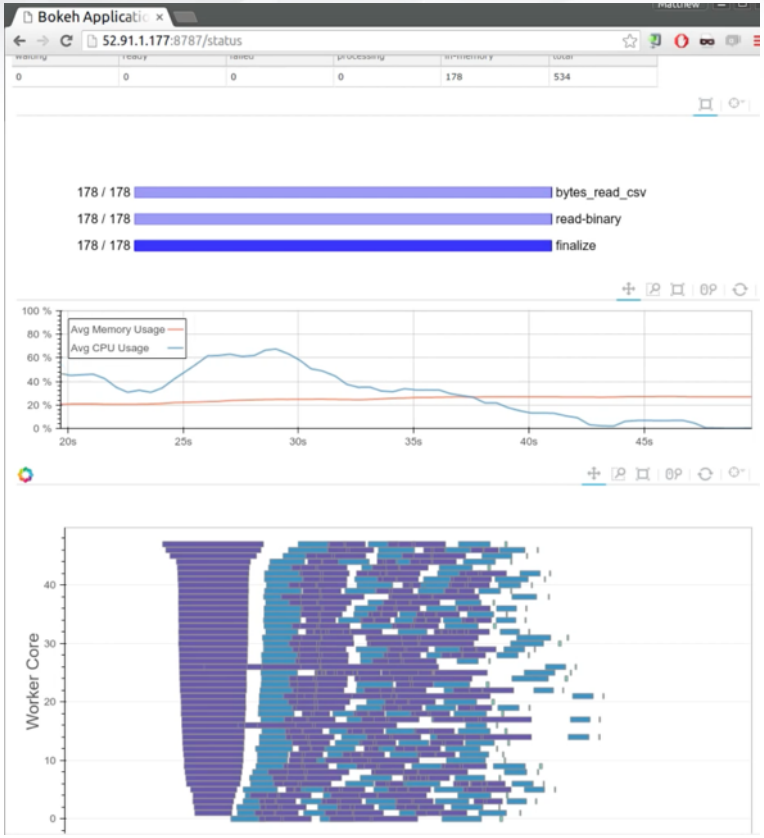
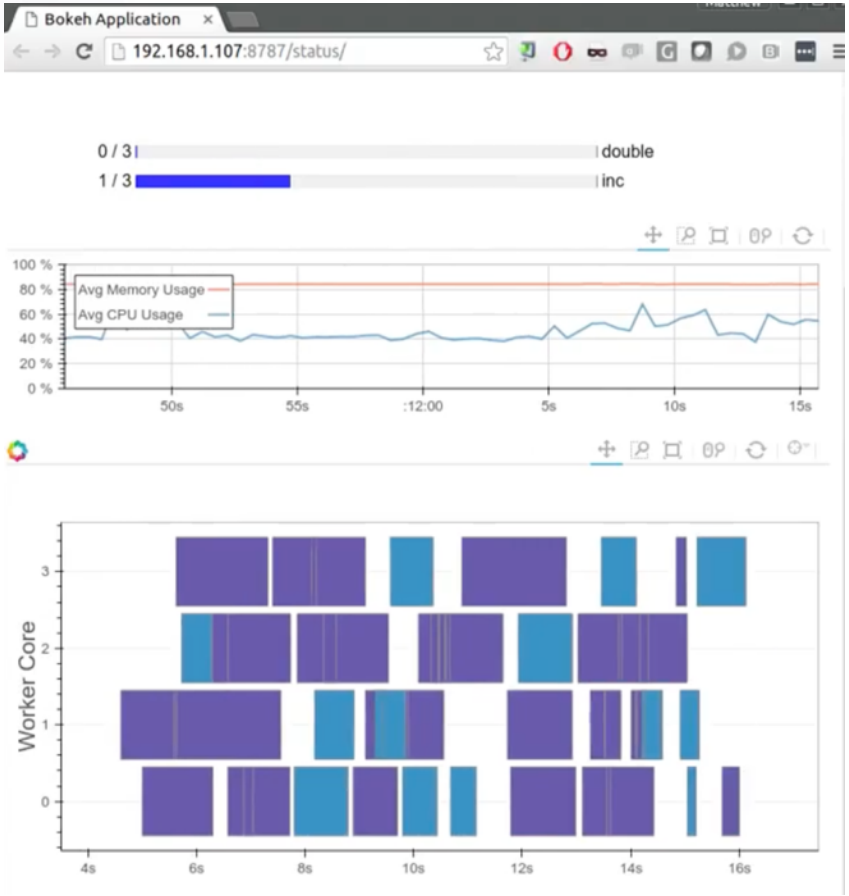




Examples

1 **Analyzing NYC Taxi CSV data using distributed Dask DataFrames**

- Demonstrate Pandas at scale
- Observe responsive user interface

2 **Distributed language processing with text data using Dask Bags**

- Explore data using a distributed memory cluster
- Interactively query data using libraries from Anaconda

3 **Analyzing global temperature data using Dask Arrays**

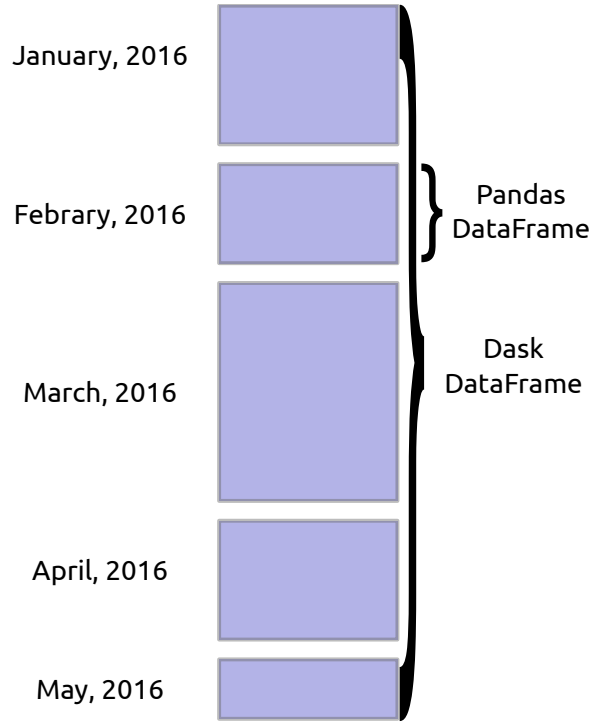
- Visualize complex algorithms
- Learn about dask collections and tasks

4 **Handle custom code and workflows using Dask Imperative**

- Deal with messy situations
- Learn about scheduling

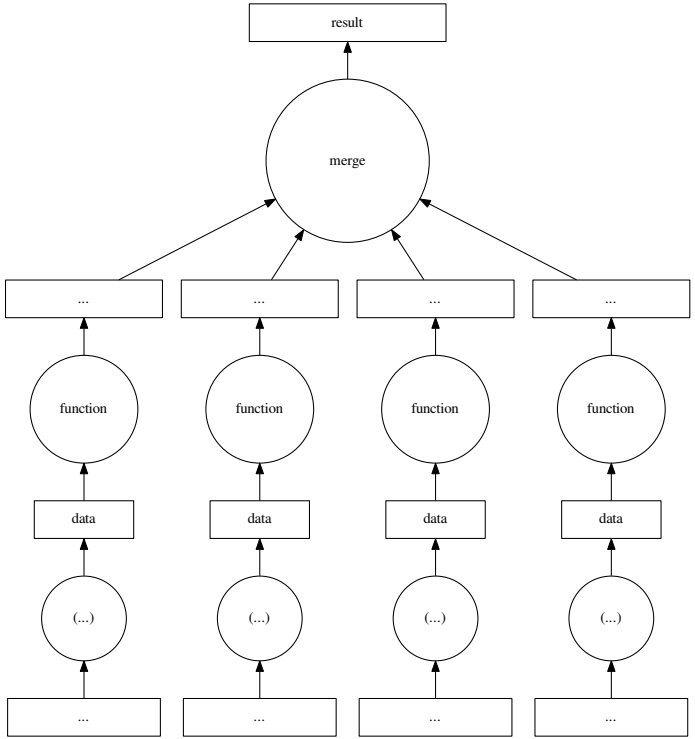
Example 1: Using Dask DataFrames on a cluster with CSV data

- Built from Pandas DataFrames
- Match Pandas interface
- Access data from HDFS, S3, local, etc.
- Fast, low latency
- Responsive user interface



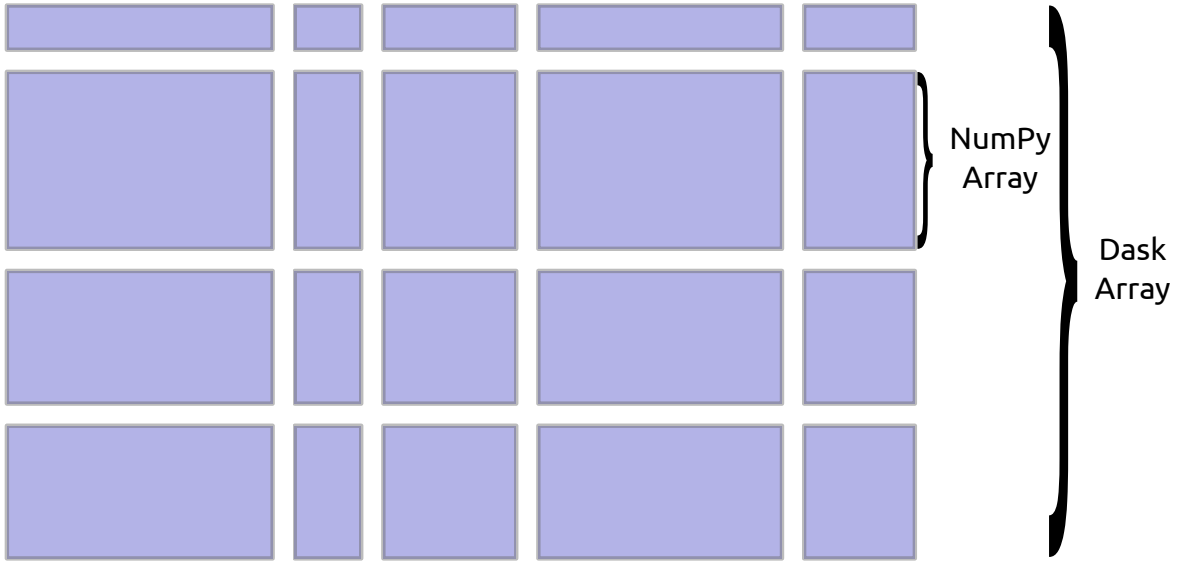
Example 2: Using Dask Bags on a cluster with text data

- Distributed natural language processing with text data stored in HDFS
- Handles standard computations
- Looks like other parallel frameworks (Spark, Hive, etc.)
- Access data from HDFS, S3, local, etc.
- Handles the common case

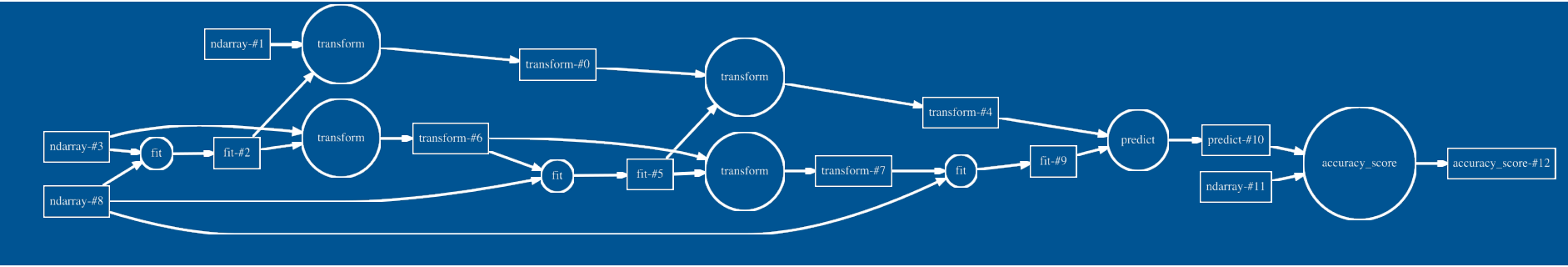


Example 3: Using Dask Arrays with global temperature data

- Built from NumPy n-dimensional arrays
- Matches NumPy interface (subset)
- Solve medium-large problems
- Complex algorithms



Example 4: Using Dask Delayed to handle custom workflows



- Manually handle functions to support messy situations
- Life saver when collections aren't flexible enough
- Combine futures with collections for best of both worlds
- Scheduler provides resilient and elastic execution

Contribute to the next stage of the journey

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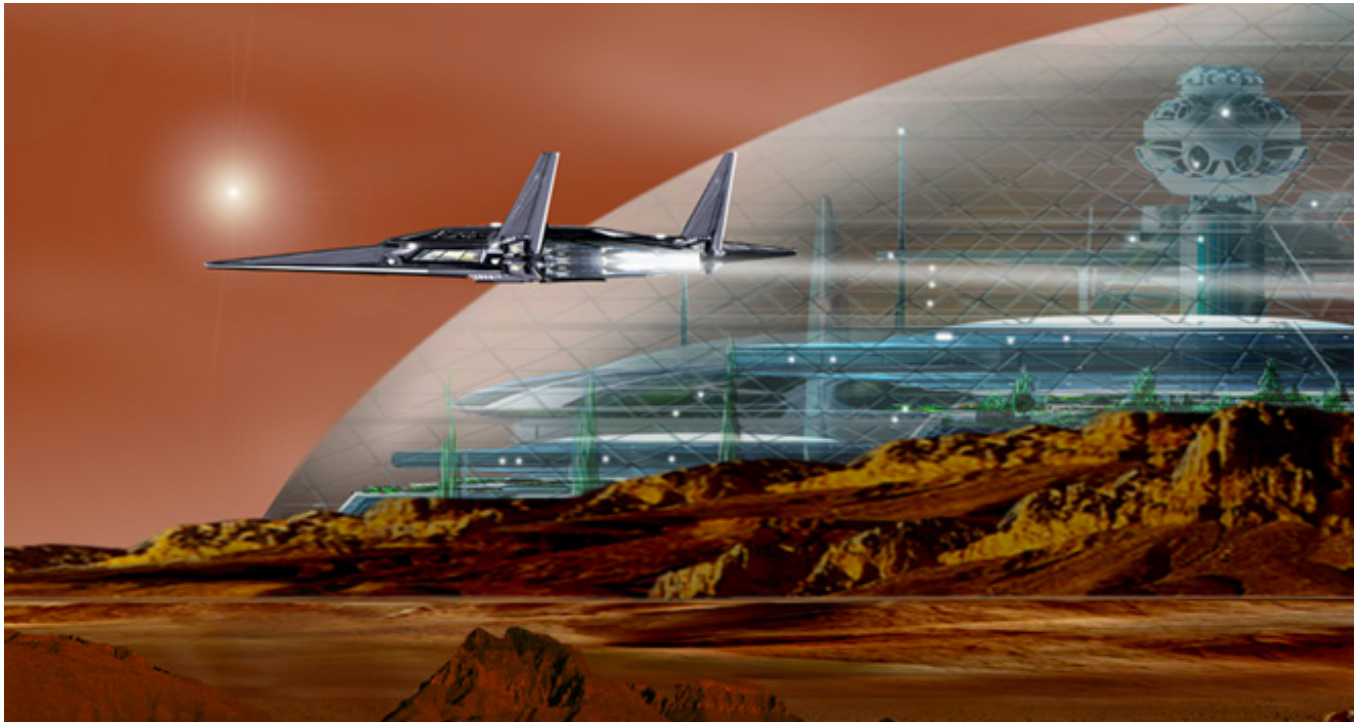
NUMFOCUS
OPEN CODE = BETTER SCIENCE

PyData



Blaze and the
Blaze ecosystem (dask, odo, dynd, datashape, data-fabric, and beyond…)