A Short History of Array Computing in Python

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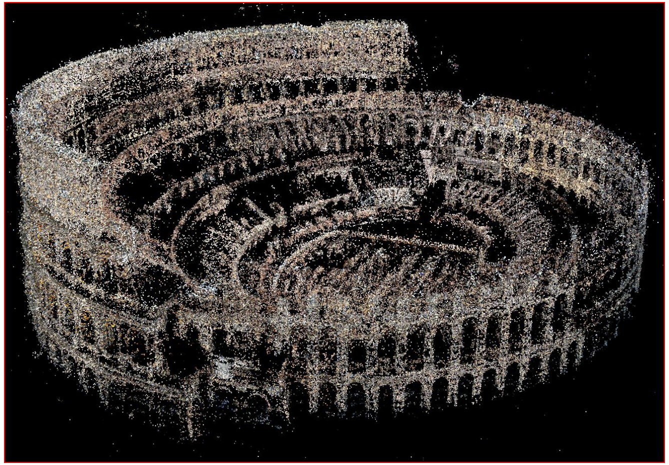
QuantStack

TOC

- Array computing in general
- History up to NumPy
- Libraries “after” NumPy
  - Pure Python libraries
  - JIT / AOT compilers
  - Deep Learning
- NumPy extension proposal

Arrays

- Used practically in all scientific domains
- Physics, Controls, Biological System, Big Data, Deep Learning, Autonomous Cars …



Array computing

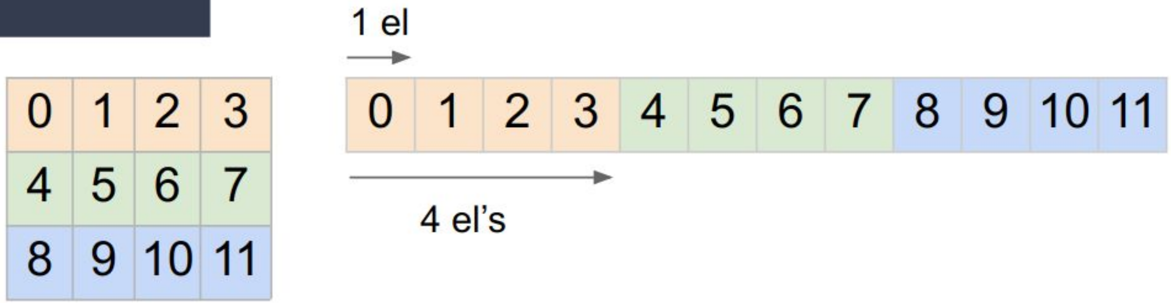
Generalize operations on scalars to … Arrays

$C \leftarrow A + B$

What is an n-dimensional Array?

- memory region (buffer)
- dimension
- shape
- Often strides

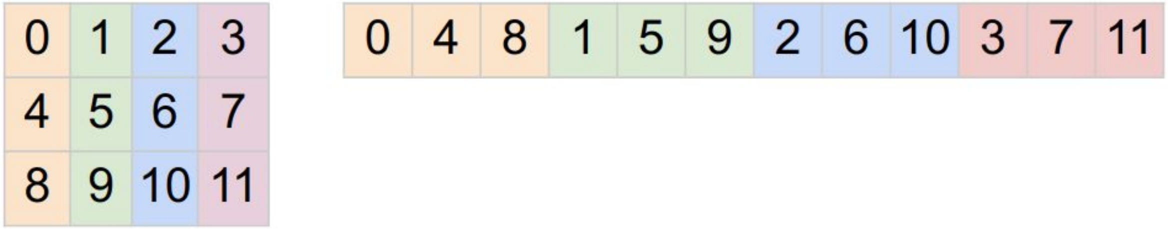
Layout	Row Major (C)
Shape	3, 4
Strides	4, 1



0	1	2	3
4	5	6	7
8	9	10	11

0	1	2	3	4	5	6	7	8	9	10	11

Layout	Col Major (F)
Shape	3, 4
Strides	1, 3



0	1	2	3
4	5	6	7
8	9	10	11

0	4	8	1	5	9	2	6	10	3	7	11

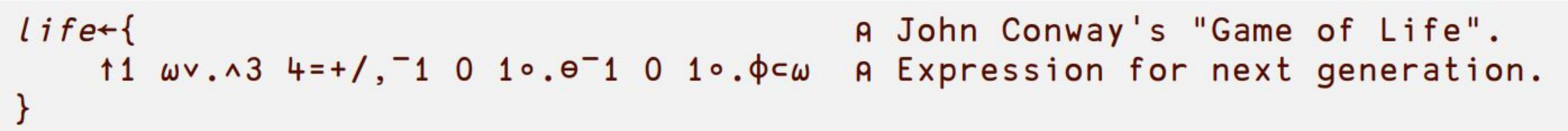
1957 / 1977 Fortran 77

- One of the oldest languages for scientific computing
- Still a reference in benchmarks
- Original implementation of BLAS & LAPACK in Fortran
- Maximum of 7 dimensions

```
integer, dimension (9, 0:99, -99:99) :: my_array
```

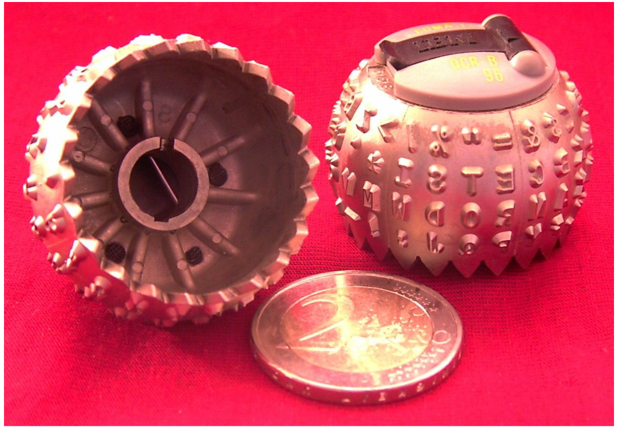
1966 APL: Honorable Mention

- Seriously *dense* language



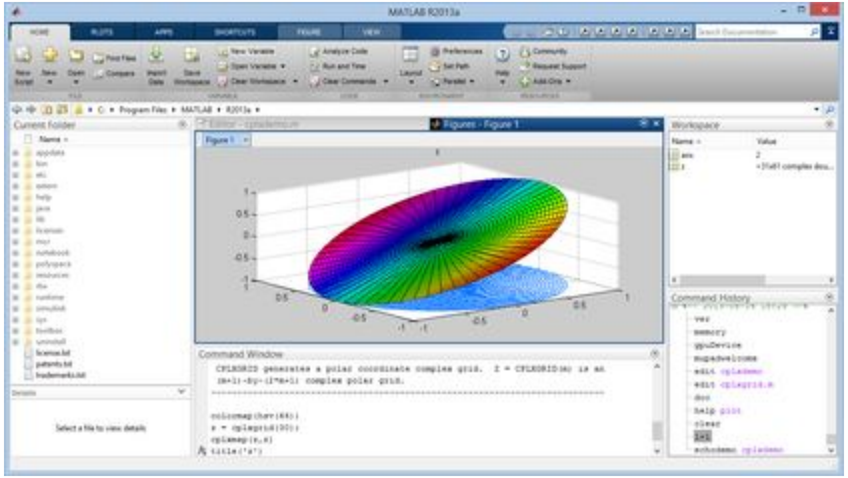
```
life←{                                ⍝ John Conway's "Game of Life".
    ↑1 ⍵∨.∧3 4=+/,¯1 0 1∘.⊖¯1 0 1∘.⌽⊂⍵  ⍝ Expression for next generation.
}
```

→ Try it online: https://tryapl.org/



1987 Matlab

- Proprietary software from Mathworks
- Dynamic interface to Fortran
- Pioneered interactive computing + visualization



1995 Numeric

- Python numerical computing package
- Inspired additions to Python (indexing syntax)

~2003 NumArray

- More flexible than Numeric
- Slower for small arrays, better for large arrays
- Split in the community:
  - SciPy remained on Numeric...

2006: NumPy

- “Merge” of Numeric and NumArray
- Fast & flexible array computing in Python
- Typed memory block
- Notion of broadcasting
- Vector Loops in C

NumPy Broadcasting

- Broadcasting: what to do when dimensions don’t match up?

NumPy ufunc

- Function that has specified input/output
- np.sin:
  - nin = 1, nout = 1
  - signature: f -> f, d -> d...
- np.add:
  - nin = 2, nout = 1
  - signature: ff -> f, dd -> d...

NumPy as a Standard

- Computing needs have shifted
- More specialized data containers needed
- Parallelization, speed, GPU, data size …

NumPy interface de-facto standard!

2007 numexpr

- Avoid temporaries
    - R = A + B + C

      -> T1 = B + C

      -> T2 = A + T1

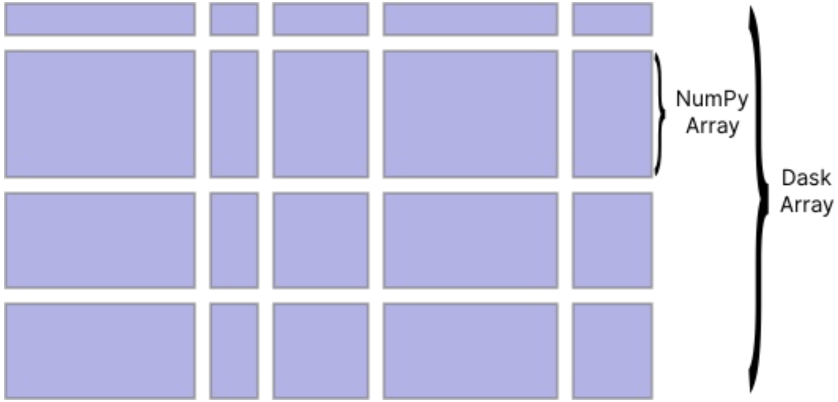
      -> R = T2
- Evaluate in chunks

2007 numexpr

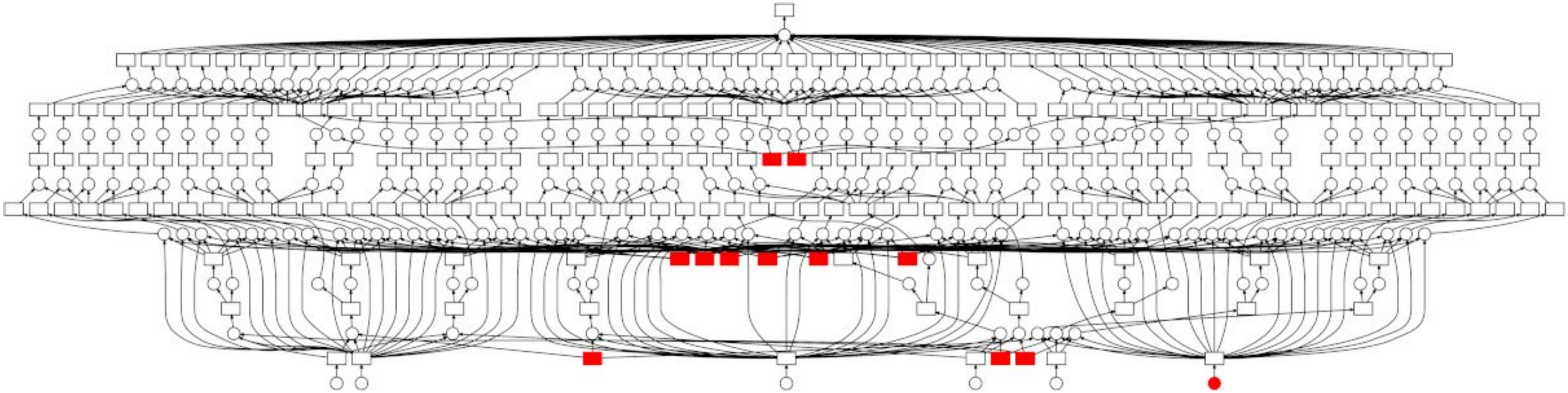
```python
import numpy as np
import numexpr as ne

a = np.arange(1e6)
b = np.arange(1e6)

ne.evaluate("a + 1")
```

2014 Dask

- Distributed array computing
- Can handle **large** data
- Execution of function distributed



2014 Dask

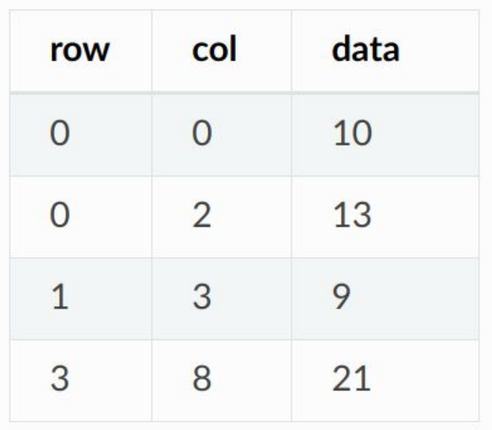


2017 pydata/sparse

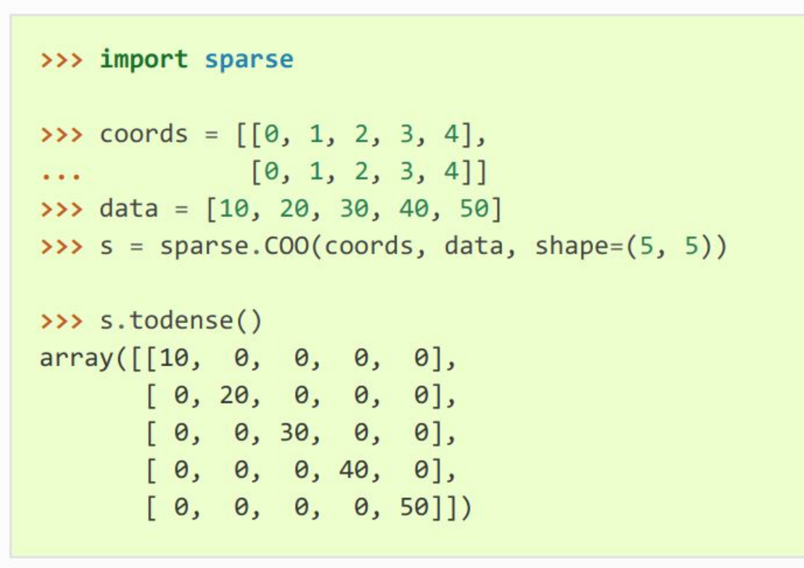
- Support for sparse ndarrays
- Advantages
  - Higher data compression
  - Faster computation
- Reuses scipy.sparse (but nD!)

2017 pydata/sparse

- Store data in COO (coordinate list) model



row	col	data
0	0	10
0	2	13
1	3	9
3	8	21



```
>>> import sparse

>>> coords = [[0, 1, 2, 3, 4],
...           [0, 1, 2, 3, 4]]
>>> data = [10, 20, 30, 40, 50]
>>> s = sparse.COO(coords, data, shape=(5, 5))

>>> s.todense()
array([[10,  0,  0,  0,  0],
       [ 0, 20,  0,  0,  0],
       [ 0,  0, 30,  0,  0],
       [ 0,  0,  0, 40,  0],
       [ 0,  0,  0,  0, 50]])
```

GPUs for computation

- Massively parallel
- Great for large data
- Cost of memory transfer from CPU → GPU
- Other programming model

2015 CuPy

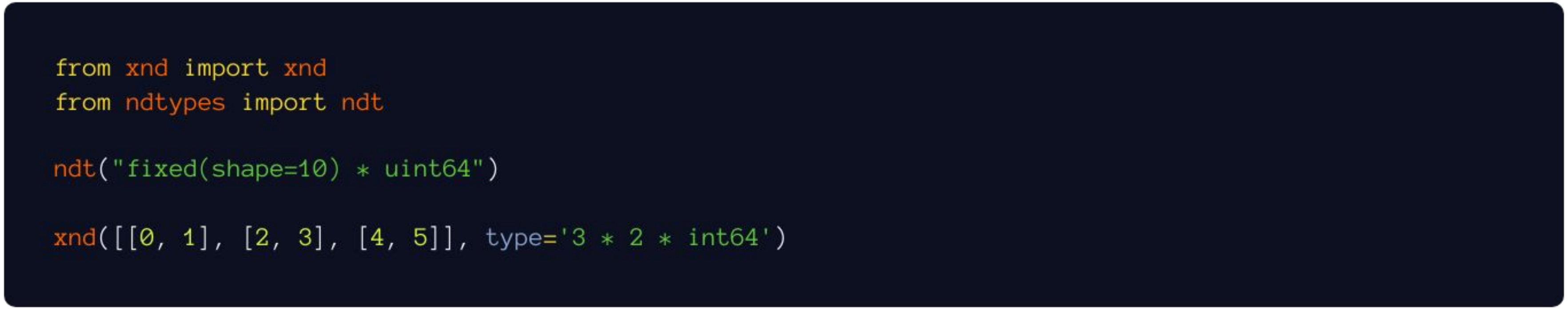
- CUDA-aware NumPy implementation
- Part of the Chainer DL framework

```
import cupy as cp
import numpy as np

a = np.arange(100)
gpu_a = cp.asarray(a)
gpu_a = gpu_a * 100

res_npy = cp.to_numpy(gpu_a)
```

2017 xnd

3 libraries:

- ndtypes: shape, type & memory
- gumath: dispatch math functions on memory container
- xnd: python bridge for typed memory



```
from xnd import xnd
from ndtypes import ndt

ndt("fixed(shape=10) * uint64")

xnd([[0, 1], [2, 3], [4, 5]], type='3 * 2 * int64')
```

JIT & AOT compilers

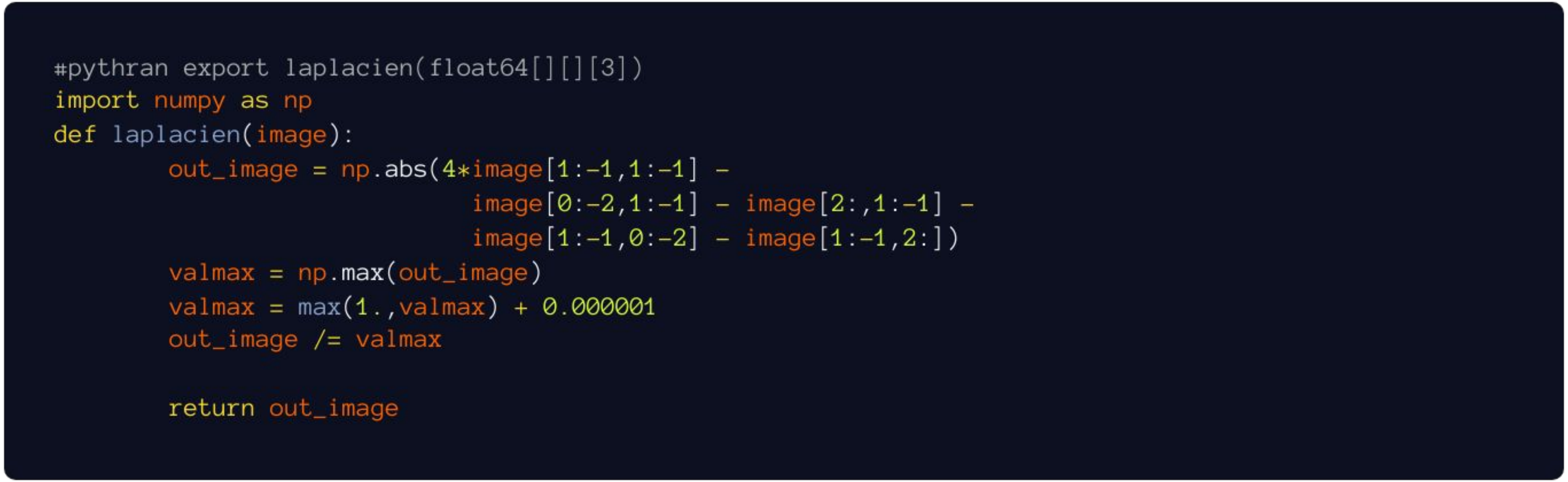
- Just in Time compilation for numeric code
- Can give incredible speed ups

2012 Pythran

- A Python/NumPy to C++ AOT compiler
- Supports high level optimizations in Python
- C++ implementation of NumPy with expression templates
- *Cython integration*

(Don’t miss the talk by Serge later today!)

2012 Pythran

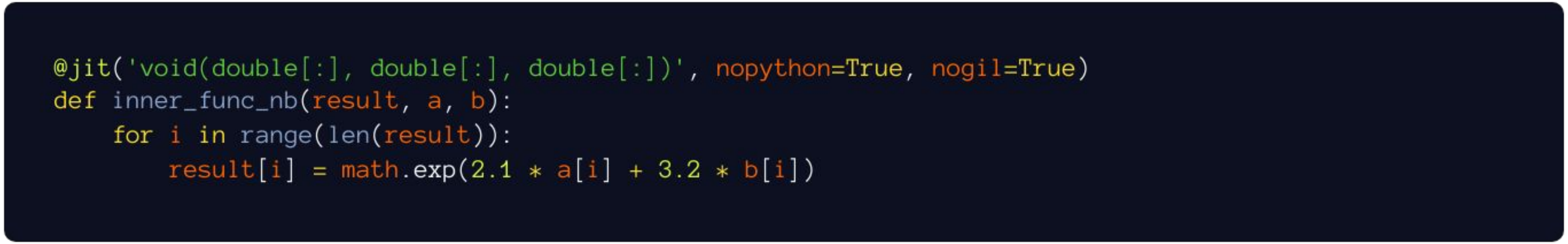


```
#pythran export laplacien(float64[][][3])
import numpy as np
def laplacien(image):
        out_image = np.abs(4*image[1:-1,1:-1] -
                             image[0:-2,1:-1] - image[2:,1:-1] -
                             image[1:-1,0:-2] - image[1:-1,2:])
        valmax = np.max(out_image)
        valmax = max(1.,valmax) + 0.000001
        out_image /= valmax

        return out_image
```

2012 Numba

- A Python to LLVM JIT
- Takes Python and compiles it to Machine Code
- GPU support (Cuda + AMD)
- For High Performance: need to write explicit “for” loops

2012 Numba



```python
@jit('void(double[:], double[:], double[:])', nopython=True, nogil=True)
def inner_func_nb(result, a, b):
    for i in range(len(result)):
        result[i] = math.exp(2.1 * a[i] + 3.2 * b[i])
```

Numba + ufunc

```
from numba import vectorize, float64

@vectorize([float64(float64, float64)])
def f(x, y):
    return x + y
```

Numba + GPU

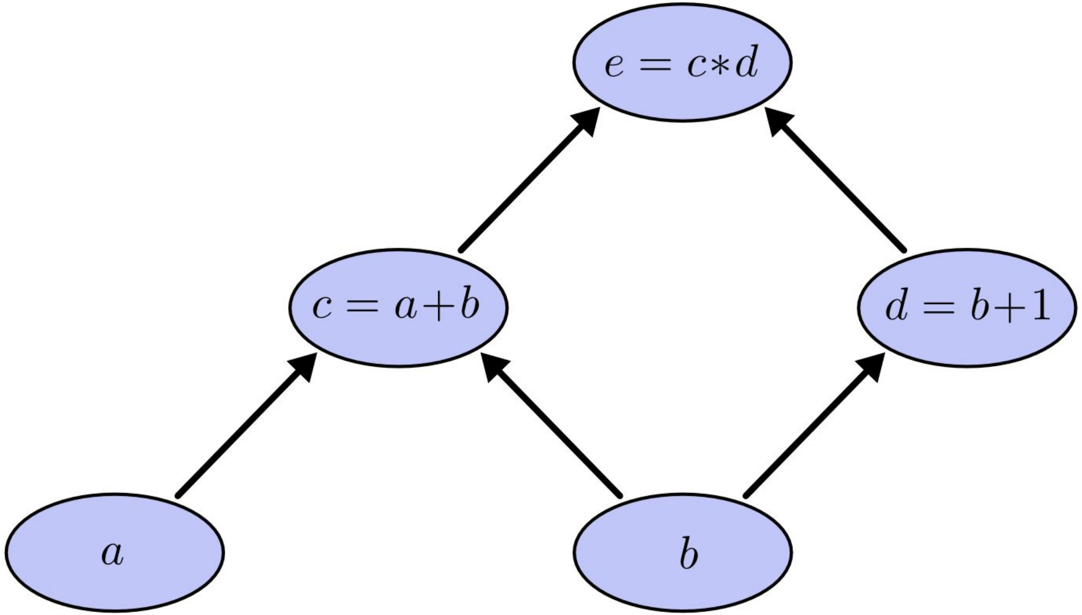
```python
@cuda.jit
def increment_a_2D_array(an_array):
    x, y = cuda.grid(2)
    if x < an_array.shape[0] and y < an_array.shape[1]:
       an_array[x, y] += 1
```

The AI winter is over …

- Deep learning revolution
- Python ecosystem benefits **heavily**
- Lot’s of array computing

Computation Graph

```
a = b = input
c = a + b
d = b + 1
e = c * d
```



Computation Graph

- Abstraction of computation
- Benefit: allows automatic differentiation
- Optimization opportunities
  - Common Subexpression Elimination
  - Algebraic simplifications: (y * x) / y → (x)
  - Constant folding (2 * 3 + a) → (6 + a)
  - Fuse ops

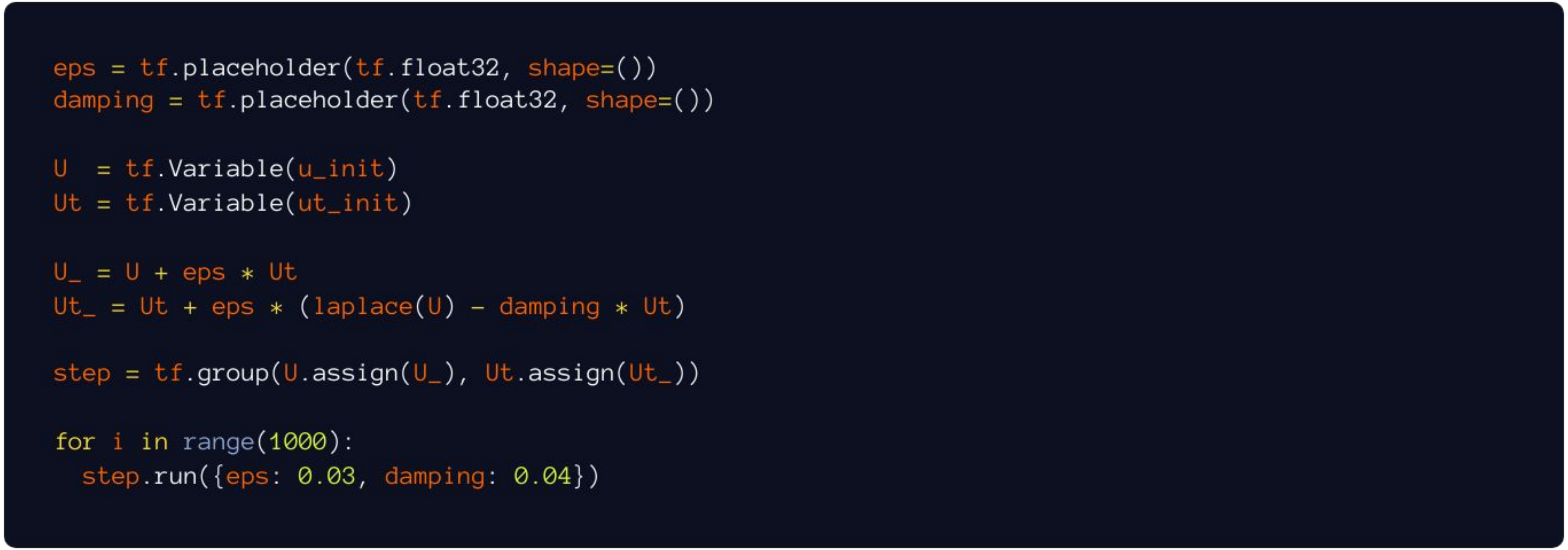
2007 Theano

- One of the first “Deep Learning” libraries
- Works on a computation graph
- Lazy evaluation
- Compiles kernels to C & CUDA

2015 TensorFlow

- Big library from Google
- Killed many others (including Theano)
- Same principle as Theano
- At the beginning: no compilation stage

2015 TensorFlow



```
eps = tf.placeholder(tf.float32, shape=())
damping = tf.placeholder(tf.float32, shape=())

U  = tf.Variable(u_init)
Ut = tf.Variable(ut_init)

U_ = U + eps * Ut
Ut_ = Ut + eps * (laplace(U) - damping * Ut)

step = tf.group(U.assign(U_), Ut.assign(Ut_))

for i in range(1000):
  step.run({eps: 0.03, damping: 0.04})
```

2015 TensorFlow + XLA

- An experimental compiler for TensorFlow graphs
- JIT + AOT modes
- Uses LLVM under the hood

2016 PyTorch

- Deep Learning Framework from Facebook
- Computation Graph, but dynamic (no deferred graph model)
- Easier to have control flow

PyTorch JIT & TorchScript

- Subset of Python that can be compiled
- Generates CUDA & CPU code

```
import torch
@torch.jit.script
def foo(x, y):
    if x.max() > y.max():
        r = x
    else:
        r = y
    return r
```

Conclusion

- NumPy is the best … API
- Many NumPy implementations
- Many downstream projects
    - Pandas
    - xarray
    - scikit-..., scipy

The array extension proposal

- 6 months ago started by M. Rocklin
- Problem: it’s hard to write generic code
- Already extension points: __array__, __array_ufunc__

```
def f(x):
    y = np.tensordot(x, x.T)
    return np.mean(np.exp(y))
```

The array extension proposal

- E.g. CuPy input → CuPy output desired
- Arguments allowed to overload __array_function__

NEP 18
numpy.org/neps/nep-0018-array-function-protocol.html

Trends

- Ecosystem has become much richer in the past years
- More compilation
- More specialized NumPy implementations
- __array_function__ will make it easy to write implementation independent code

Thanks

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- Questions?

xtensor

python

Check out xtensor & xtensor-python

NumPy for C++ ;)

Follow me on Twitter @wuoulf or GitHub @wolfv

NumPy ufunc

- Automatic broadcasting
- ufunc supports:
  - __call__
  - reduce
  - reduceat
  - accumulate
  - outer
  - inner