



# Introduction to Numerical Computing with Numpy

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# Introduction to Numerical Computing with Numpy

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# Introduction to Numerical Computing with NumPy

SciPy Conference Tutorial  
2022



## NumPy

The Standard Numerical Library  
for Python

# Syllabus



1. Introducing Arrays
2. Indexing and Slicing
3. Creating Arrays
4. Array Calculations
5. The Array Data Structure
6. Structure Operations



a = 

0	1	2	3
---	---	---	---

# NumPy

Introducing Arrays

# Introducing NumPy Arrays

## SIMPLE ARRAY CREATION

```
>>> a = np.array([0, 1, 2, 3])
>>> a
array([0, 1, 2, 3])
```

## CHECKING THE TYPE

```
>>> type(a)
numpy.ndarray
```

## NUMERIC "TYPE" OF ELEMENTS

```
>>> a.dtype
dtype('int32')
```

## NUMBER OF DIMENSIONS

```
>>> a.ndim
1
```

## ARRAY SHAPE

```
# Shape returns a tuple listing the
# length of the array along each
# dimension.
>>> a.shape
(4,)
```

## BYTES PER ELEMENT

```
>>> a.itemsize
4
```

## BYTES OF MEMORY USED

```
# Return the number of bytes used by
# the data portion of the array.
>>> a.nbytes
16
```

# Array Operations

## SIMPLE ARRAY MATH

```
>>> a = np.array([1, 2, 3, 4])
>>> b = np.array([2, 3, 4, 5])
>>> a + b
array([3, 5, 7, 9])
```

```
>>> a * b
array([ 2, 6, 12, 20])
```

```
>>> a ** b
array([ 1,  8, 81, 1024])
```


## MATH FUNCTIONS

```
# create array from 0.0 to 10.0
>>> x = np.arange(11.0)
```

```
# multiply entire array by scalar
# value
>>> c = (2.0 * np.pi) / 10.0
>>> c
0.62831853071795862
>>> c * x
array([0.    , 0.628, ..., 6.283])
```

```
# in-place operations
>>> x *= c
>>> x
array([0.    , 0.628, ..., 6.283])
```

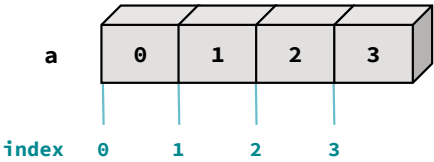
```
# apply functions to array
>>> y = np.sin(x)
```

 NumPy defines these constants:  
pi = 3.14159265359  
e = 2.71828182846

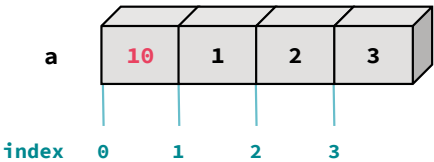
# Setting Array Elements

## ARRAY INDEXING

```
>>> a[0]
0
```



```
>>> a[0] = 10
>>> a
array([10, 1, 2, 3])
```



## BEWARE OF TYPE COERCION

```
>>> a.dtype
dtype('int32')

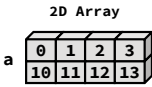
# assigning a float into an int32
# array truncates the decimal part
>>> a[0] = 10.6
>>> a
array([10, 1, 2, 3])

# fill has the same behavior
>>> a.fill(-4.8)
>>> a
array([-4, -4, -4, -4])
```

# Multi-Dimensional Arrays

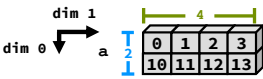
## MULTI-DIMENSIONAL ARRAYS

```
>>> a = np.array([[ 0, 1, 2, 3],
...               [10,11,12,13]])
>>> a
array([[ 0, 1, 2, 3],
       [10,11,12,13]])
```



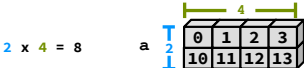
## SHAPE – (ROWS, COLUMNS)

```
>>> a.shape
(2, 4)
```



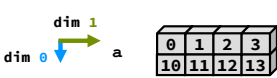
## ELEMENT COUNT

```
>>> a.size
8
```



## NUMBER OF DIMENSIONS

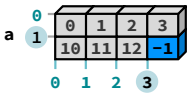
```
>>> a.ndim
2
```



## ARRAY SHAPE

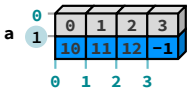
```
>>> a[1, 3]
13

>>> a[1, 3] = -1
>>> a
array([[ 0, 1, 2, 3],
       [10,11,12,-1]])
```



## ADDRESS SECOND (ONETH) ROW USING SINGLE INDEX

```
>>> a[1]
array([10, 11, 12, -1])
```



# Formatting Numeric Display

## DEFAULT FORMATTING

```
>>> a = np.arange(1.0, 3.0, 0.5)
>>> a
array([1. , 1.5, 2. , 2.5])

>>> a * np.pi
array([3.14159265, 4.71238898, 6.28318531,
       7.85398163])

>>> a * np.pi * 1e8
array([3.14159265e+08, 4.71238898e+08,
       6.28318531e+08, 7.85398163e+08])

>>> a * np.pi * 1e-6
array([3.14159265e-06, 4.71238898e-06,
       6.28318531e-06, 7.85398163e-06])
```

## USER FORMATTING

```
# set precision
>>> np.set_printoptions(
    precision=2)

>>> a
array([1. , 1.5, 2. , 2.5])

>>> a * np.pi
array([3.14, 4.71, 6.28, 7.85])

>>> a * np.pi * 1e8
array([3.14e+08, 4.71e+08, 6.28e+08,
       7.85e+08])

>>> a * np.pi * 1e-6
array([3.14e-06, 4.71e-06, 6.28e-06,
       7.85e-06])

# suppress scientific notation
>>> np.set_printoptions(
    suppress=True)

>>> a * np.pi * 1e-6
array([0., 0., 0., 0.])
```



	0	1	2	3	4	5
0	0	1	2	3	4	5
1	10	11	12	13	14	15
2	20	21	22	23	24	25
3	30	31	32	33	34	35
4	40	41	42	43	44	45
5	50	51	52	53	54	55

# NumPy

Indexing and Slicing



# Slicing

`var[lower:upper:step]`

- Extracts a portion of a sequence by specifying a lower and upper bound.
- The lower-bound element is included, but the upper-bound element is **not** included.
- Mathematically: [lower, upper). The step value specifies the stride between elements.

## SLICING ARRAYS

```
#           -5 -4 -3 -2 -1
# indices:  0  1  2  3  4
>>> a = np.array([10,11,12,13,14])

# [10, 11, 12, 13, 14]
>>> a[1:3]
array([11, 12])

# negative indices work also
>>> a[1:-2]
array([11, 12])
>>> a[-4:3]
array([11, 12])
```

## OMITTING INDICES

```
# omitted boundaries are assumed to be
# the beginning (or end) of the array

# grab first three elements
>>> a[:3]
array([10, 11, 12])

# grab last two elements
>>> a[-2:]
array([13, 14])

# every other element
>>> a[::2]
array([10, 12, 14])
```

# Array Slicing

## SLICING WORKS MUCH LIKE STANDARD PYTHON SLICING

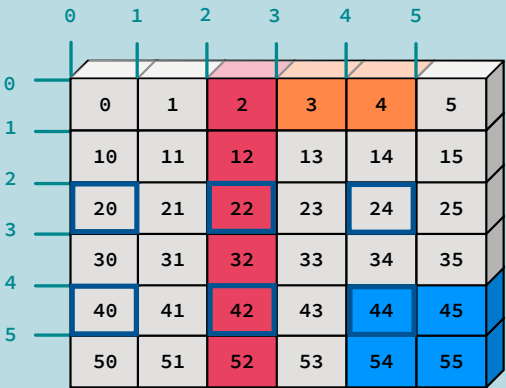
```
>>> a[0, 3:5]
array([3, 4])

>>> a[4:, 4:]
array([[44, 45],
       [54, 55]])

>>> a[:, 2]
array([2, 12, 22, 32, 42, 52])
```

## SLICING ARRAYS

```
>>> a[2::2, ::2]
array([[20, 22, 24],
       [40, 42, 44]])
```



# Assigning to a Slice

Slices are references to locations in memory.

These memory locations can be used in assignment operations.

```
>>> a = np.array([0, 1, 2, 3, 4])  
  
# slicing the last two elements returns the data there  
>>> a[-2:]  
array([3, 4])  
  
# we can insert an iterable of length two  
>>> a[-2:] = [-1, -2]  
>>> a  
array([0, 1, 2, -1, -2])  
  
# or a scalar value  
>>> a[-2:] = 99  
>>> a  
array([0, 1, 2, 99, 99])
```

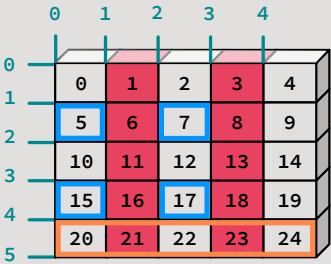
# Give it a try!



Create the array below with the command

```
a = np.arange(25).reshape(5, 5)
```

and extract the slices as indicated.



# Sliced Arrays Share Data

Arrays created by slicing share data with the originating array.  
Changing values in a slice also changes the original array.

```
>>> a = np.array([0, 1, 2, 3, 4])

# create a slice containing two elements of a
>>> b = a[2:4]
>>> b
array([2, 3])
>>> b[0] = 10

# changing b changed a!
>>> a
array([ 0,  1, 10,  3,  4])
>>> np.shares_memory(a, b)
True
```

# Fancy Indexing

## INDEXING BY POSITION

```
>>> a = np.arange(0, 80, 10)

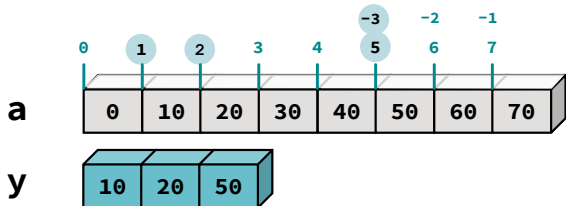
# fancy indexing
>>> indices = [1, 2, -3]
>>> y = a[indices]
>>> y
array([10, 20, 50])

# this also works with setting
>>> a[indices] = 99
>>> a
array([0, 99, 99, 30, 40, 99, 60, 70])
```

## INDEXING WITH BOOLEANS

```
# manual creation of masks
>>> mask = np.array(
...     [0, 1, 1, 0, 0, 1, 0, 0],
...     dtype=bool)

# fancy indexing
>>> y = a[mask]
>>> y
array([99, 99, 99])
```



## Fancy Indexing in 2-D

```
>>> a[[0, 1, 2, 3, 4],  
...   [1, 2, 3, 4, 5]]  
array([ 1, 12, 23, 34, 45])
```

```
>>> a[3:, [0, 2, 5]]  
array([[30, 32, 35],  
       [40, 42, 45],  
       [50, 52, 55]])
```

```
>>> mask = np.array(  
...     [1, 0, 1, 0, 0, 1],  
...     dtype=bool)  
>>> a[mask, 2]  
array([2, 22, 52])
```

	0	1	2	3	4	5
0	0	1	2	3	4	5
1	10	11	12	13	14	15
2	20	21	22	23	24	25
3	30	31	32	33	34	35
4	40	41	42	43	44	45
5	50	51	52	53	54	55



Unlike slicing, fancy indexing creates copies instead of a view into original array.

## Give it a try!

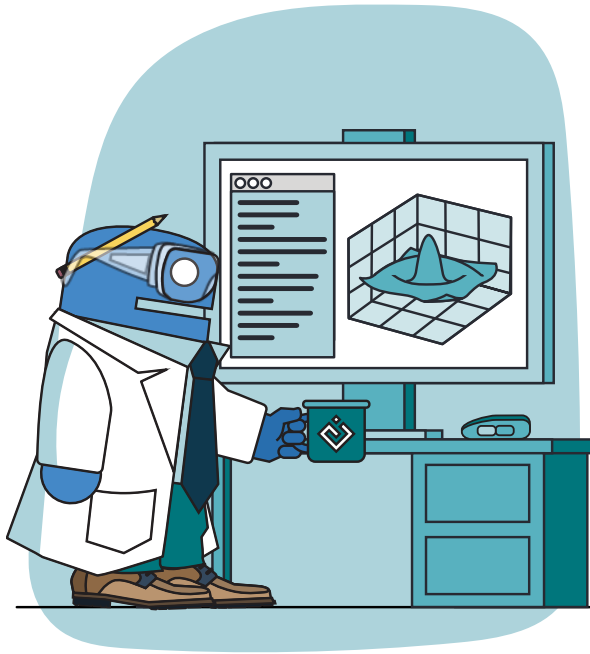


1. Create the array below with

```
a = np.arange(25).reshape(5, 5)  
and extract the elements indicated in blue.
```

2. Extract all the numbers divisible by 3 using a boolean mask.

	0	1	2	3	4
0	0	1	2	3	4
1	5	6	7	8	9
2	10	11	12	13	14
3	15	16	17	18	19
4	20	21	22	23	24



```
OOO
arange()
linspace()
array()
zeros()
ones()
```

# NumPy

## Creating Arrays

## Array Constructor Examples

### FLOATING POINT ARRAYS

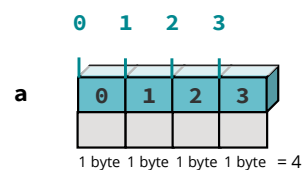
```
# Default to double precision
>>> a = np.array([0,1.0,2,3])
>>> a.dtype
dtype('float64')
>>> a.nbytes
32
```

### REDUCING PRECISION

```
>>> a = np.array([0,1.,2,3],
...               dtype='float32')
>>> a.dtype
dtype('float32')
>>> a.nbytes
16
```

### ARRAY SHAPE

```
>>> a = np.array([0,1,2,3],
...               dtype='uint8')
>>> a.dtype
dtype('uint8')
>>> a.nbytes
4
```



Base 2	Base 10
00000000	-> 0 = 0*2**0 + 0*2**1 + ... + 0*2**7
00000001	-> 1 = 1*2**0 + 0*2**1 + ... + 0*2**7
00000010	-> 2 = 0*2**0 + 1*2**1 + ... + 0*2**7
...	
11111111	-> 255 = 1*2**0 + 1*2**1 + ... + 1*2**7

# Array Creation Functions

ARANGE

ONES, ZEROS

**arange([start,] stop[, step], dtype=None)**

Nearly identical to Python's **range()**. Creates an array of values in the range [start,stop) with the specified step value. Allows non-integer values for start, stop, and step. Default **dtype** is derived from the start, stop, and step values.

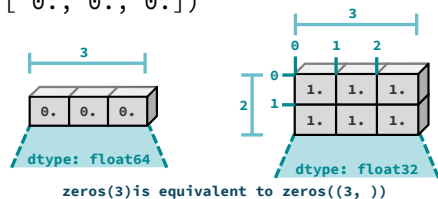
```
>>> np.arange(4)
array([0, 1, 2, 3])
>>> np.arange(0, 2*pi, pi/4)
array([ 0.000, 0.785, 1.571, 2.356, 3.142,
        3.927, 4.712, 5.497])
```

```
# Be careful...
>>> np.arange(1.5, 2.1, 0.3)
array([ 1.5, 1.8, 2.1])
```

**ones(shape, dtype='float64')**  
**zeros(shape, dtype='float64')**

**shape** is a number or sequence specifying the dimensions of the array. If **dtype** is not specified, it defaults to **float64**.

```
>>> np.ones((2, 3),
...         dtype='float32')
array([[ 1.,  1.,  1.],
       [ 1.,  1.,  1.]])
>>> np.zeros(3)
array([ 0.,  0.,  0.])
```



# Array Creation Functions (cont'd)

IDENTITY

EMPTY AND FULL

```
# Generate an n by n identity array.
# The default dtype is float64.
>>> a = np.identity(4)
>>> a
array([[ 1.,  0.,  0.,  0.],
       [ 0.,  1.,  0.,  0.],
       [ 0.,  0.,  1.,  0.],
       [ 0.,  0.,  0.,  1.]])
>>> a.dtype
dtype('float64')
>>> np.identity(4, dtype=int)
array([[ 1,  0,  0,  0],
       [ 0,  1,  0,  0],
       [ 0,  0,  1,  0],
       [ 0,  0,  0,  1]])
```

```
# empty(shape, dtype=float64,
#        order='C')
>>> np.empty(2)
array([1.78021120e-306,
       6.95357225e-308])

# array filled with 5.0
>>> a = np.full(2, 5.0)
array([5.,  5.])

# alternative approaches
# (slower)
>>> a = np.empty(2)
>>> a.fill(4.0)
>>> a
array([4.,  4.])
>>> a[:] = 3.0
>>> a
array([3.,  3.])
```

# Array Creation Functions (cont'd)



## Linspace

# Generate N evenly spaced elements  
# between (and including) start and  
# stop values.

```
>>> np.linspace(0, 1, 5)
array([0., 0.25, 0.5, 0.75, 1.0])
```

## Logspace

# Generate N evenly spaced elements on  
# a log scale between base\*\*start and  
# base\*\*stop (default base=10)

```
>>> np.logspace(0, 1, 5)
array([1., 1.78, 3.16, 5.62, 10.])
```

## Arrays from/to text files

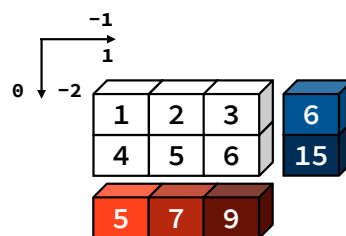
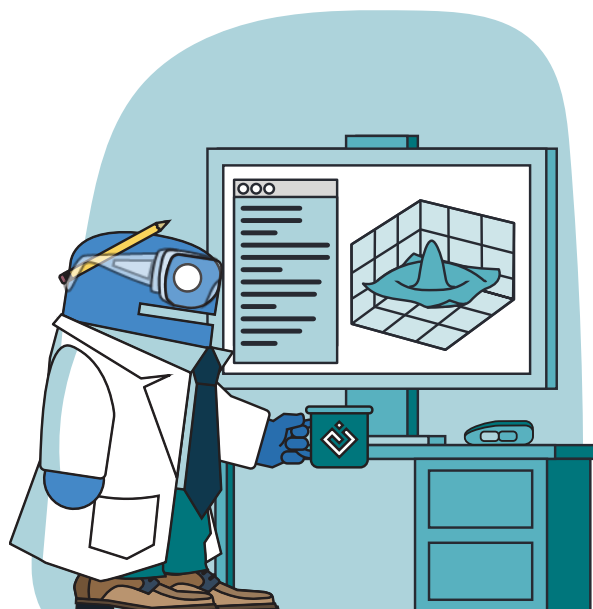
```
BEGINNING OF THE FILE
% Day, Month, Year, Skip, Avg Power
01, 01, 2000, x876, 13 % crazy day!
% we don't have Jan 03rd
04, 01, 2000, xfed, 55
```

Data.txt

# loadtxt() automatically generates an  
# array from the txt file

```
arr = np.loadtxt('Data.txt',
...             skiprows=1,
...             dtype=int, delimiter=",",
...             usecols = (0,1,2,4),
...             comments = "%")
```

# Save an array into a txt file  
np.savetxt('filename.txt', arr)



# NumPy

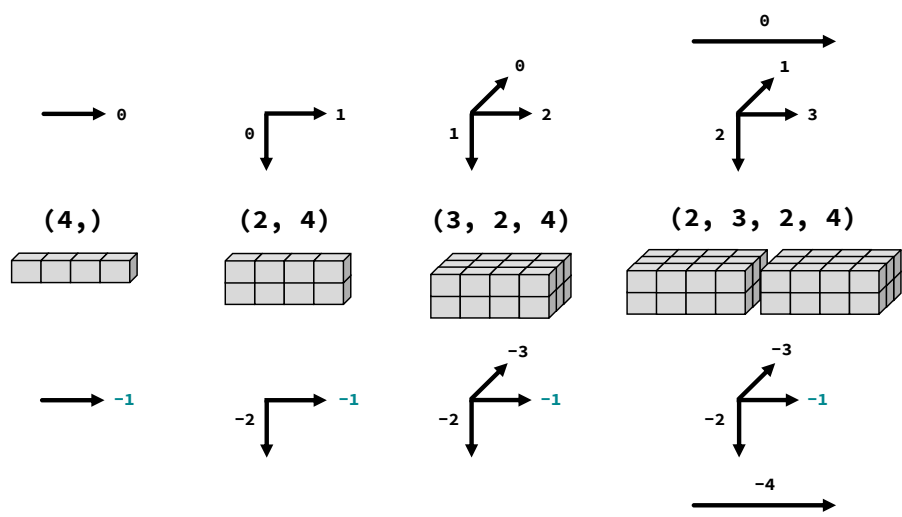
Array Calculation Methods

# Computations with Arrays

Rule 1:	Operations between multiple array objects are first checked for proper shape match.
Rule 2:	Mathematical operators (+ - * / exp, log, ...) apply element by element, on the values.
Rule 3:	Reduction operations (mean, std, skew, kurt, sum, prod, ...) apply to the whole array, unless an axis is specified.
Rule 4:	Missing values propagate unless explicitly ignored (nanmean, nansum, ...).

# Multi-Dimensional Arrays

## VISUALIZING MULTI-DIMENSIONAL ARRAYS





# Array Calculation Methods

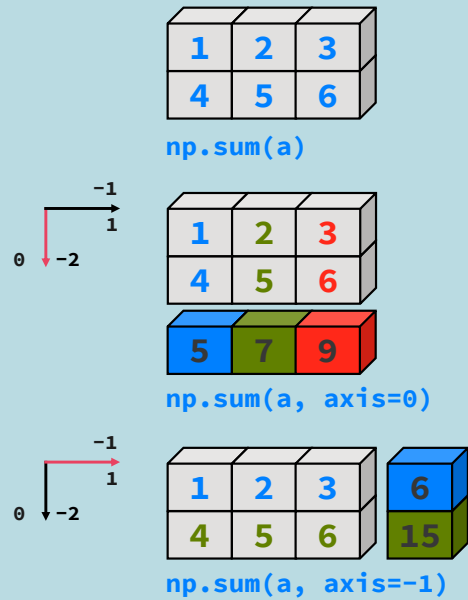
## SUM METHOD

```
# Methods act on data stored in the array
>>> a = np.array([[1,2,3],
                  [4,5,6]])

# .sum() defaults to adding up all the
# values in an array.
>>> a.sum()
21

# supply the keyword axis to sum along the
# 0th axis
>>> a.sum(axis=0)
array([5, 7, 9])

# supply the keyword axis to sum along the
# last axis
>>> a.sum(axis=-1)
array([ 6, 15])
```



# Other Operations on Arrays

## SUM FUNCTION

```
# Functions work on data passed to it
>>> a = np.array([[1,2,3],
                  [4,5,6]])

# sum() defaults to adding up all
# values in an array.
>>> np.sum(a)
21

# supply an axis argument to sum along
# a specific axis
>>> np.sum(a, axis=0)
array([5, 7, 9])
```

## OTHER METHODS AND FUNCTIONS

### Mathematical functions

- `sum`, `prod`
- `min`, `max`, `argmin`, `argmax`
- `ptp` (max – min)

### Statistics

- `mean`, `std`, `var`

### Truth value testing

- `any`, `all`

See the NumPy appendix for more.

# Min/Max

## MIN

```
>>> a = np.array([[2, 3], [0, 1]])
# Prefer NumPy functions to builtins when
# working with arrays
>>> np.min(a)
0
# Most NumPy reducers can be used as
# methods as well as functions
>>> a.min()
0
```

## MAX

```
# Use the axis keyword to find max values
# for one dimension
>>> a.max(axis=0)
array([2, 3])
# as a function
>>> np.max(a, axis=1)
array([3, 1])
```

## ARGMIN/MAX

```
# Many tasks (like optimization) are
# interested in the location of a min/max,
# not the value
>>> a.argmax()
1
# arg methods return the location in a 1D,
# flattened version of the original array
>>> np.argmin(a)
2
```

## UNRAVELING

```
# NumPy includes a function to un-flatten
# 1D locations
>>> np.unravel_index(
...     a.argmax(), a.shape)
(0, 1)
```

# Where



## COORDINATE LOCATIONS

```
# NumPy's where function has two
# distinct uses. One is to provide
# coordinates from masks.
>>> a = np.arange(-2, 2) ** 2
>>> a
array([4, 1, 0, 1])
>>> mask = a % 2 == 0
>>> mask
array([ True, False,  True, False])

# Coordinates are returned as a tuple
# of arrays, one for each axis.
>>> np.where(mask)
(array([0, 2]),)
```

## CONDITIONAL ARRAY CREATION

```
# Where can also be used to construct a new
# array by choosing values from other
# arrays of the same shape.
>>> positives = np.arange(1, 5)
>>> negatives = -positives
>>> np.where(mask, positives,
...         negatives)
array([1, -2, 3, -4])

# Or from scalar values. This can be useful
# for recoding arrays.
>>> np.where(mask, 1, 0)
array([1, 0, 1, 0])

# Or from both.
>>> np.where(mask, positives, 0)
array([1, 0, 3, 0])
```

# Statistics Array Methods

MEAN

```
>>> a = np.array([[1,2,3],
...               [4,5,6]])

# mean value of each column
>>> a.mean(axis=0)
array([ 2.5,  3.5,  4.5])
>>> np.mean(a, axis=0)
array([ 2.5,  3.5,  4.5])
```

STANDARD DEV./VARIANCE

```
# Standard Deviation
>>> a.std(axis=0)
array([ 1.5,  1.5,  1.5])
# For sample, set ddof=1
>>> a.std(axis=0, ddof=1)
array([ 2.12,  2.12,  2.12])

# variance
>>> a.var(axis=0)
array([2.25, 2.25, 2.25])
>>> np.var(a, axis=0)
array([2.25, 2.25, 2.25])
```

## Give it a try!



Create the array below with

```
a = np.arange(-15, 15).reshape(5, 6) ** 2
```

and compute:

- 1. The maximum of each row
- 2. The mean of each column
- 3. The position of the overall minimum

	0	1	2	3	4	5
0	225	196	169	144	121	100
1	81	64	49	36	25	16
2	9	4	1	0	1	4
3	9	16	25	36	49	64
4	81	100	121	144	169	196



a			+	b			=	y		
0	0	0		0	1	2		0	1	2
10	10	10		0	1	2		10	11	12
20	20	20		0	1	2		20	21	22
30	30	30		0	1	2		30	31	32

# NumPy

## Array Broadcasting

## Array Broadcasting

NumPy arrays of different dimensionality can be combined in the same expression. Arrays with smaller dimension are **broadcasted** to match the larger arrays, *without copying data*.

Broadcasting has **two rules**.

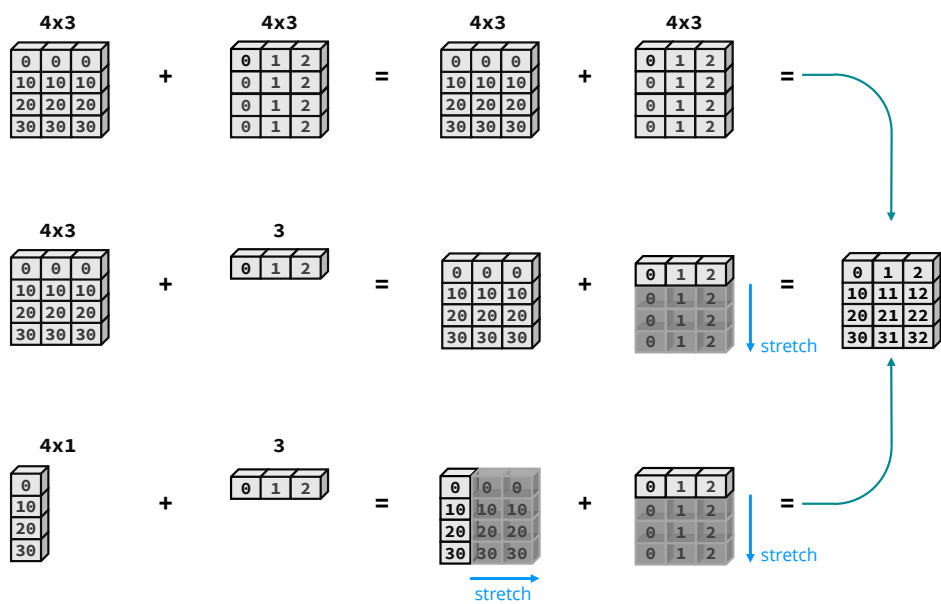
### RULE 1: PREPEND ONES TO SMALLER ARRAY'S SHAPE

```
>>> import numpy as np
>>> a = np.ones((3, 5)) # a.shape == (3, 5)
>>> b = np.ones((5,)) # b.shape == (5,)
>>> b.reshape(1, 5) # result is a (1,5)-shaped array
>>> b[np.newaxis, :] # equivalent, more concise
```

### RULE 2: DIMENSIONS OF SIZE 1 ARE REPEATED WITHOUT COPYING

```
>>> c = a + b # c.shape == (3, 5)
# is logically equivalent to...
>>> tmp_b = b.reshape(1, 5)
>>> tmp_b_repeat = tmp_b.repeat(3, axis=0)
>>> c = a + tmp_b_repeat
# But broadcasting makes no copies of "b"s data!
```

# Array Broadcasting

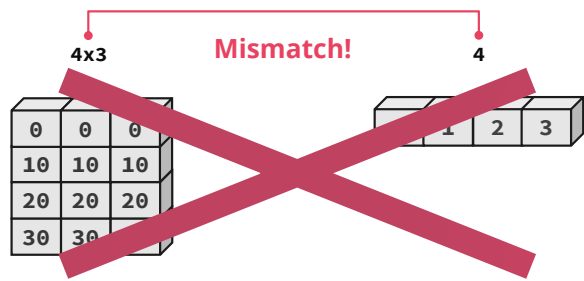


# Broadcasting Rules

The **trailing axes** of either arrays **must be 1 or both must have the same size** for broadcasting to occur.

Otherwise, a

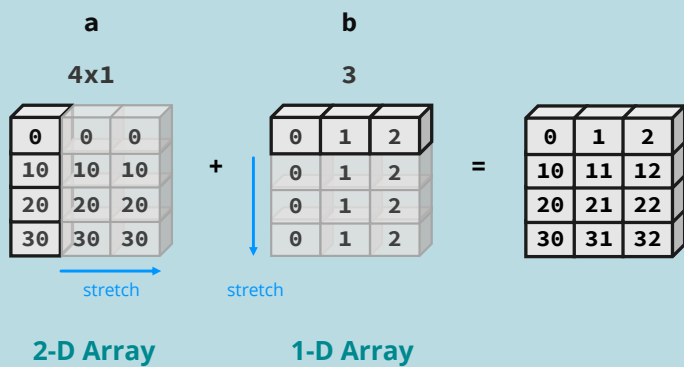
**"ValueError: shape mismatch: objects cannot be broadcast to a single shape"** exception is thrown.



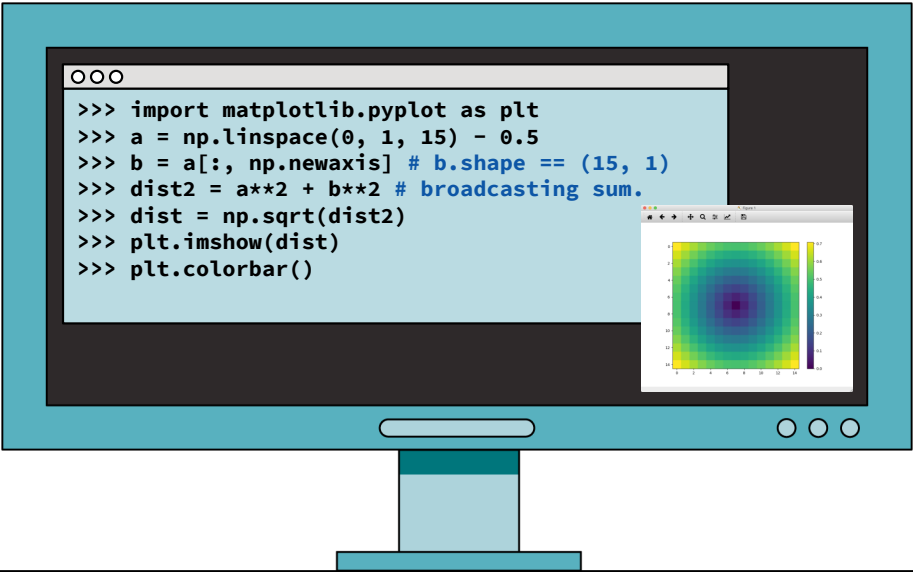


# Broadcasting in Action

```
>>> a = array([0, 10, 20, 30])
>>> b = array([0, 1, 2])
>>> y = a[:, newaxis] + b
```



# Application: Distance from Center



# Broadcasting's Usefulness

Broadcasting can often be used to replace needless data replication inside a NumPy array expression.

`np.meshgrid()` – use **newaxis** appropriately in broadcasting expressions.

`np.repeat()` – broadcasting makes repeating an array along a dimension of size 1 unnecessary.

## MESHGRID: COPIES DATA

```
>>> x, y = \
...     np.meshgrid([1,2],
...                  [3,4,5])
>>> z = x + y
```

## BROADCASTING: NO COPIES

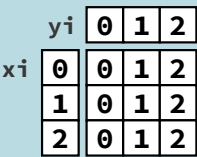
```
>>> x = np.array([1, 2])
>>> y = np.array([3, 4, 5])
>>> z = x[np.newaxis, :] \
...       + y[:, np.newaxis]
```

# Broadcasting Indices

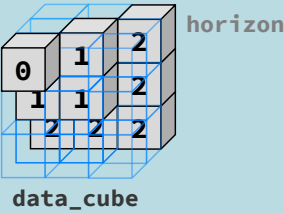
Broadcasting can also be used to **slice elements from different “depths”** in a 3-D (or any other shape) array. This is a very powerful feature of indexing.

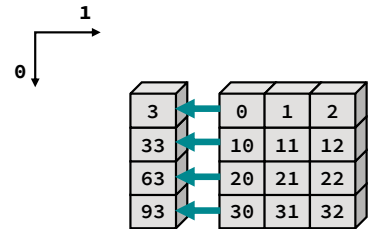
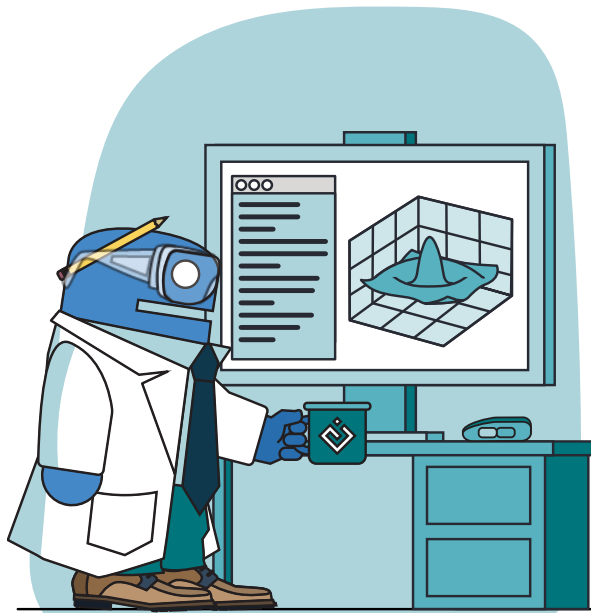
```
>>> data_cube = np.arange(27).reshape(3, 3, 3)
>>> yi, xi = np.meshgrid(np.arange(3), np.arange(3),
...                       sparse=True)
>>> zi = np.array([[0, 1, 2],
...                 [1, 1, 2],
...                 [2, 2, 2]])
>>> horizon = data_cube[xi, yi, zi]
```

## Indices



## Selected Data





# NumPy

Universal Function Methods

## Universal Function Methods

The mathematical, comparative, logical, and bitwise operators *op* that take two arguments (binary operators) have special methods that operate on arrays:

```
>>> op.reduce(a,axis=0)
>>> op.accumulate(a,axis=0)
>>> op.outer(a,b)
>>> op.reduceat(a,indices)
```



# op.reduce()

**op.reduce(a)** applies **op** to all the elements in a 1-D array **a** reducing it to a single value.

For example:

y = add.reduce(a)

$$= \sum_{n=0}^{N-1} a[n]$$

$$= a[0] + a[1] + \dots + a[N-1]$$

## ADD EXAMPLE

```
>>> a = np.array([1,2,3,4])
>>> np.add.reduce(a)
10
```

## STRING LIST EXAMPLE

```
>>> a = np.array(['ab','cd','ef'],
...               dtype='object')
>>> np.add.reduce(a)
'abcdef'
```

## LOGICAL OP EXAMPLES

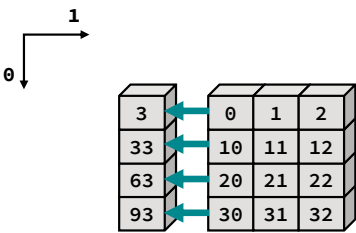
```
>>> a = np.array([1,1,0,1])
>>> np.logical_and.reduce(a)
False
>>> np.logical_or.reduce(a)
True
```

# op.reduce()

For multidimensional arrays, **op.reduce(a,axis)** applies **op** to the elements of **a** along the specified **axis**. The resulting array has dimensionality one less than **a**. The default value for **axis** is 0.

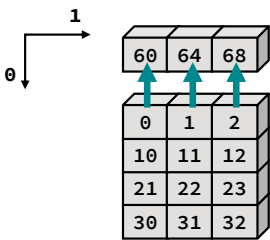
## SUMMING UP EACH ROW

```
>>> a = np.arange(3) + np.arange(0, 40,
...               10).reshape(-1, 1)
>>> np.add.reduce(a,1)
array([ 3, 33, 63, 93])
```



## SUM COLUMNS BY DEFAULT

```
>>> np.add.reduce(a)
array([60, 64, 68])
```



# op.accumulate()

**op.accumulate(a)** creates a new array containing the intermediate results of the **reduce** operation at each element in **a**.

For example:

y = add.accumulate(a)

$$= \left[ \sum_{n=0}^0 a[n], \sum_{n=0}^1 a[n], \dots, \sum_{n=0}^{N-1} a[n] \right]$$

## ADD EXAMPLE

```
>>> a = np.array([1,2,3,4])
>>> np.add.accumulate(a)
array([ 1,  3,  6, 10])
```

## STRING LIST EXAMPLE

```
>>> a = np.array(['ab','cd','ef'],
...               dtype='object')
>>> np.add.accumulate(a)
array(['ab','abcd','abcdef'],
      dtype=object)
```

## LOGICAL OP EXAMPLES

```
>>> a = np.array([1,1,0])
>>> np.logical_and.accumulate(a)
array([True, True, False])
>>> np.logical_or.accumulate(a)
array([True, True, True])
```

# op.reduceat()

**op.reduceat(a,indices)** applies **op** to ranges in the 1-D array **a** defined by the values in **indices**. The resulting array has the same length as **indices**.

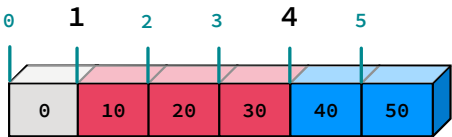
For example:

y = add.reduceat(a, indices)

$$y[i] = \sum_{n=indices[i]}^{indices[i+1]} a[n]$$

## EXAMPLE

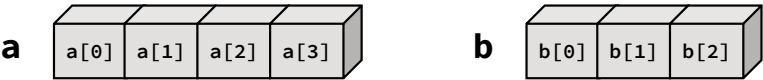
```
>>> a = np.array([0,10,20,30,40,50])
>>> indices = np.array([1,4])
>>> np.add.reduceat(a,indices)
array([60, 90])
```



For multidimensional arrays, **reduceat()** is always applied along the last axis (sum of rows for 2-D arrays). This is different from the default for **reduce()** and **accumulate()**.

# op.outer()

**op.outer(a,b)** forms all possible combinations of elements between **a** and **b** using **op**. The shape of the resulting array results from concatenating the shapes of **a** and **b**. (Order matters.)



```
>>> np.add.outer(a,b)
```

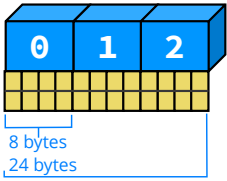
a[0]+b[0]	a[0]+b[1]	a[0]+b[2]
a[1]+b[0]	a[1]+b[1]	a[1]+b[2]
a[2]+b[0]	a[2]+b[1]	a[2]+b[2]
a[3]+b[0]	a[3]+b[1]	a[3]+b[2]

```
>>> np.add.outer(b,a)
```

b[0]+a[0]	b[0]+a[1]	b[0]+a[2]	b[0]+a[3]
b[1]+a[0]	b[1]+a[1]	b[1]+a[2]	b[1]+a[3]
b[2]+a[0]	b[2]+a[1]	b[2]+a[2]	b[2]+a[3]



Memory Block

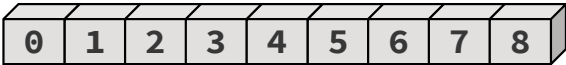


# NumPy

The Array Data Structure

# Array Data Structure

Memory Block



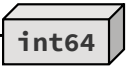
Python View:



# Array Data Structure

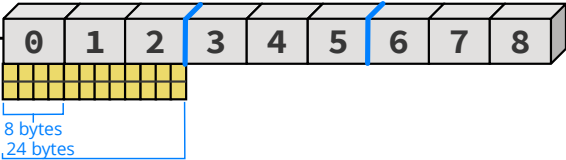
NDArray Data Structure

dtype	*	
ndim	2	
shape	3	3
strides	24	8
data	*	

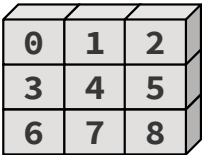


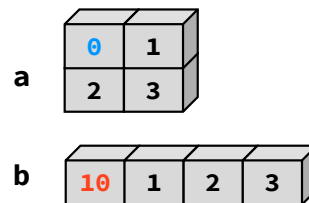
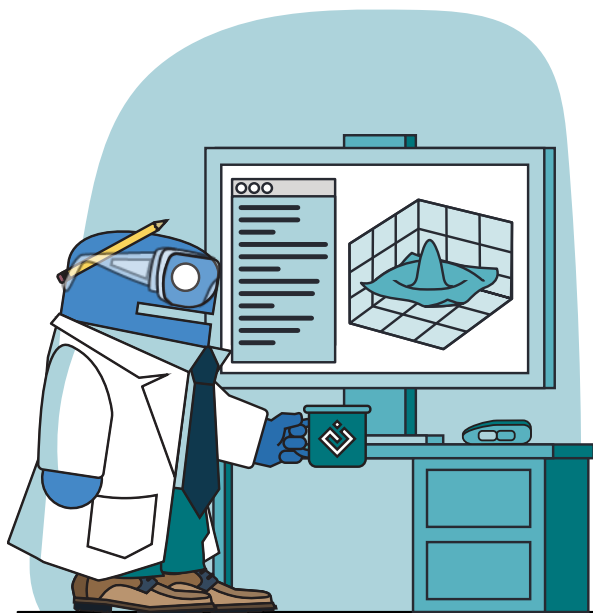
The int64 data type describes the array data elements

Memory Block



Python View:





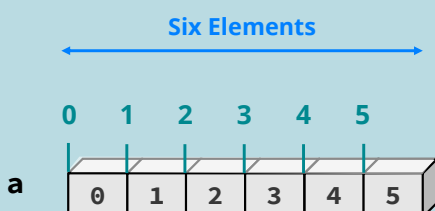
# NumPy

## Structure Operations

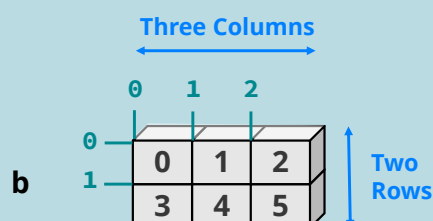
## Operations on the Array Structure

Operations that only affect the array structure, not the data, can usually be executed without copying memory.

```
>>> a = np.arange(6)
>>> a
```



```
>>> b = a.reshape(2, 3)
>>> b
```



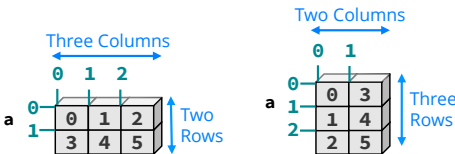
This **is not** a new copy of the data.  
The original data **does not** get reordered.

# Transpose

## TRANPOSE

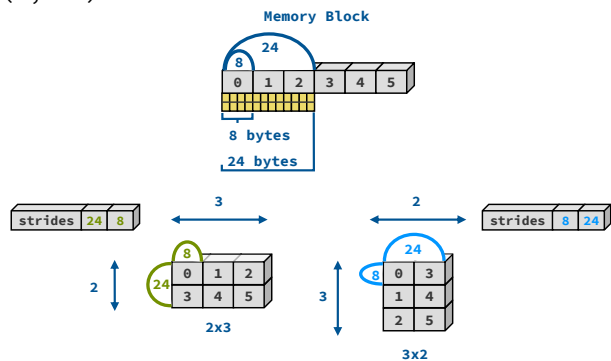
```
>>> a = np.array([[0,1,2],
...               [3,4,5]])
>>> a.shape
(2,3)

# Transpose swaps the order of axes.
>>> a.T
array([[0, 3],
       [1, 4],
       [2, 5]])
>>> a.T.shape
(3,2)
```



## TRANPOSE RETURNS VIEWS

```
# Transpose does not move values around in
# memory. It only changes the order of
# "strides" in the array
>>> a.strides
(24, 8)
>>> a.T.strides
(8, 24)
```



# Reshaping Arrays

## RESHAPE

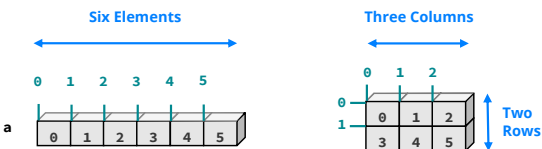
```
>>> a = np.array([[0,1,2],
...               [3,4,5]])
# Return a new array with a different shape
# (a view where possible)
>>> a.reshape(3,2)
array([[0, 1],
       [2, 3],
       [4, 5]])

# Reshape cannot change the number of
# elements in an array
>>> a.reshape(4,2)
ValueError: total size of new array must be
unchanged
```

## SHAPE

```
>>> a = np.arange(6)
>>> a
array([0, 1, 2, 3, 4, 5])
>>> a.shape
(6,)

# Reshape array in-place to 2x3
>>> a.shape = (2,3)
>>> a
array([[0, 1, 2],
       [3, 4, 5]])
```



# Flattening Arrays

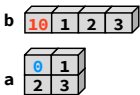
## FLATTEN (SAFE)

**a.flatten()** converts a multi-dimensional array into a 1-D array. The new array is a copy of the original data.

```
# Create a 2D array
>>> a = np.array([[0,1],
...               [2,3]])

# Flatten out elements to 1D
>>> b = a.flatten()
>>> b
array([0,1,2,3])

# Changing b does not change a
>>> b[0] = 10
>>> b
array([10,1,2,3])
>>> a
array([[0, 1],
       [2, 3]])
```

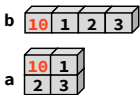


## RAVEL (EFFICIENT)

**a.ravel()** is the same as **a.flatten()**, but returns a reference (or view) of the array if possible (i.e., the memory is contiguous). Otherwise the new array copies the data. **np.ravel()** can be applied to non-array objects.

```
# Flatten out elements to 1-D
>>> b = a.ravel()
>>> b
array([0,1,2,3])

# Changing b does change a
>>> b[0] = 10
>>> b
array([10,1,2,3])
>>> a
array([[10, 1],
       [ 2, 3]])
```



# Stay in touch!



Enthought



Enthought Media



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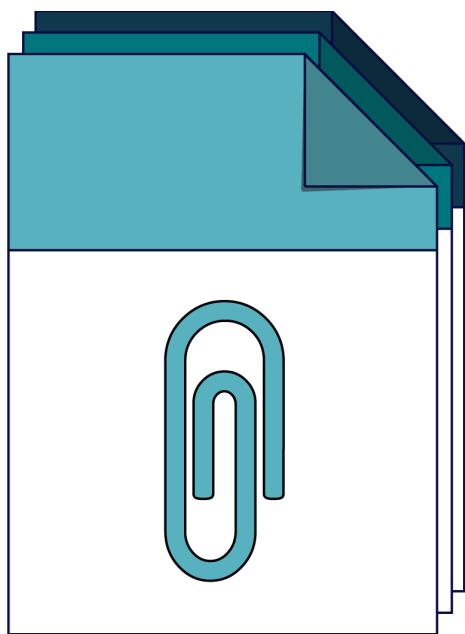


SciPy



EuroSciPy

Please complete the online survey!  
(link on course web page)



# Appendix

Additional Material

**Enthought powers  
digital transformation  
for science.**



# We Partner with Industry Leaders















Confidential and Proprietary 59

ABOUT ENTHOUGHT

# Foundation for Success

- Global, privately-owned company with headquarters in Austin
- Offices in Houston, Texas; Cambridge, United Kingdom; Zürich, Switzerland; and Tokyo, Japan
- Deep roots in the Python community of scientists and engineers
- 80% of employees have graduate degrees or PhDs in science and engineering

# Partner with Enthought



**Science is at the core of your business. And ours.**

Designed by scientists, for scientists



**The Enthought Approach is proven.**

Catalyzing innovation by transforming technology, people, and processes



**We're at the intersection of science and technology.**

Deep scientific expertise and computational knowledge



**We empower scientists.**

Equipping scientists with digital skills and technology

