Arkouda

αρκούδα

NumPy-like arrays at massive scale!

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Why?

- “Python is the new bash”

- We have data analyses which need to be done at a much larger scale… because sampling to run at smaller scale alters what can be seen in the data

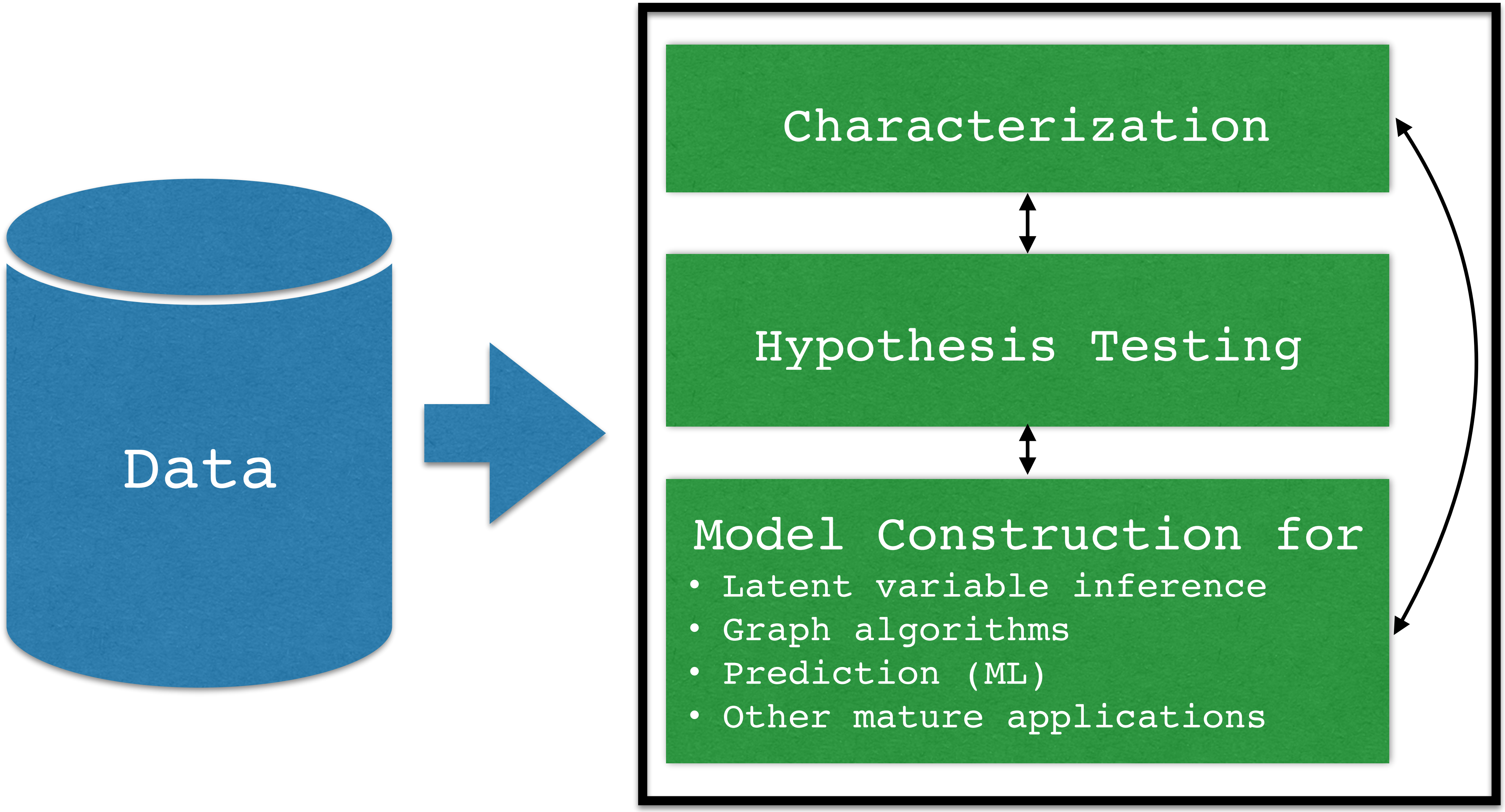
- We need to enable our data scientists with tools they know… so why not co-opt an interface or two

- Because we can and it’s fun!

We want some
of our
Data
Scientists
to drive
an F22!

Jupyter allows
Data
Scientists
to drive a
cool plane!

Data Science Workflow



Data

Characterization

Hypothesis Testing

Model Construction for

- Latent variable inference
- Graph algorithms
- Prediction (ML)
- Other mature applications

Principles: stay in memory (interactive)
and use packages

Goal: NumPy for HPC

- Distributed arrays with parallel primitives
- Familiar, interactive interface
- Smooth integration with mature HPC code

Why Python/NumPy API?

- NumPy is pervasive across Jupiter Notebooks
- Python data science packages communicate via NumPy arrays
- NumPy arrays wrap C and Fortran code for heavy lifting
- Need similar integration point for distributed HPC code!

Approach

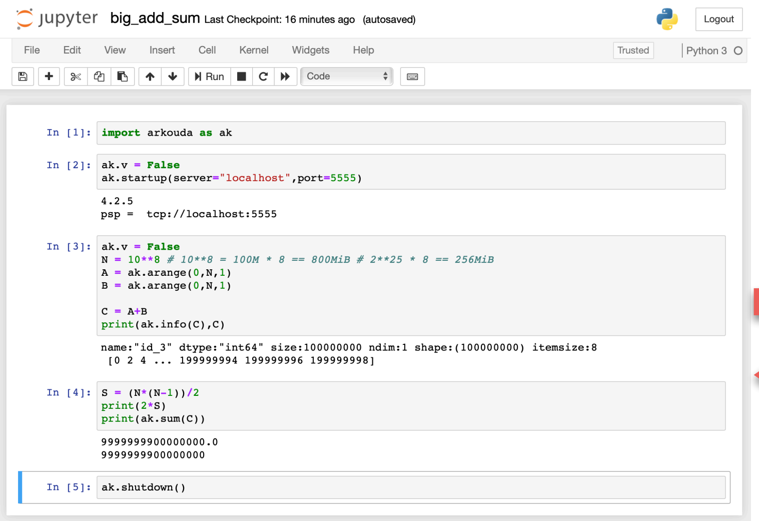
- Other efforts approach from the interactive/interpreted side
- We decided to approach from the HPC side
- Nobody that we knew of was starting with HPC-level performance and working towards interactivity
- Preserving as close to interactive speed as we can

What?

- Present the user with a familiar interface
- Allow different execution contexts to coexist and communicate
    - A single threaded context: Python3
    - A multithreaded and distributed context: Chapel
- Work without users knowing about all the HPC stuff
- Currently a very targeted definition to allow specific analyses to be done

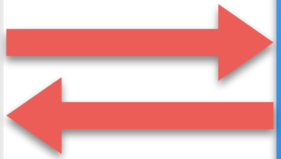
Structure

Jupyter/Python3



```
In [1]: import arkouda as ak

In [2]: ak.v = False
        ak.startup(server="localhost",port=5555)

        4.2.5
        psp =  tcp://localhost:5555

In [3]: ak.v = False
        N = 10**8 # 10**8 = 100M * 8 == 800MiB # 2**25 * 8 == 256MiB
        A = ak.arange(0,N,1)
        B = ak.arange(0,N,1)

        C = A+B
        print(ak.info(C),C)

        name:"id_3" dtype:"int64" size:100000000 ndim:1 shape:(100000000) itemsize:8
         [0 2 4 ... 199999994 199999996 199999998]

In [4]: S = (N*(N-1))/2
        print(2*S)
        print(ak.sum(C))

        9999999900000000.0
        9999999900000000

In [5]: ak.shutdown()
```

ØMQ



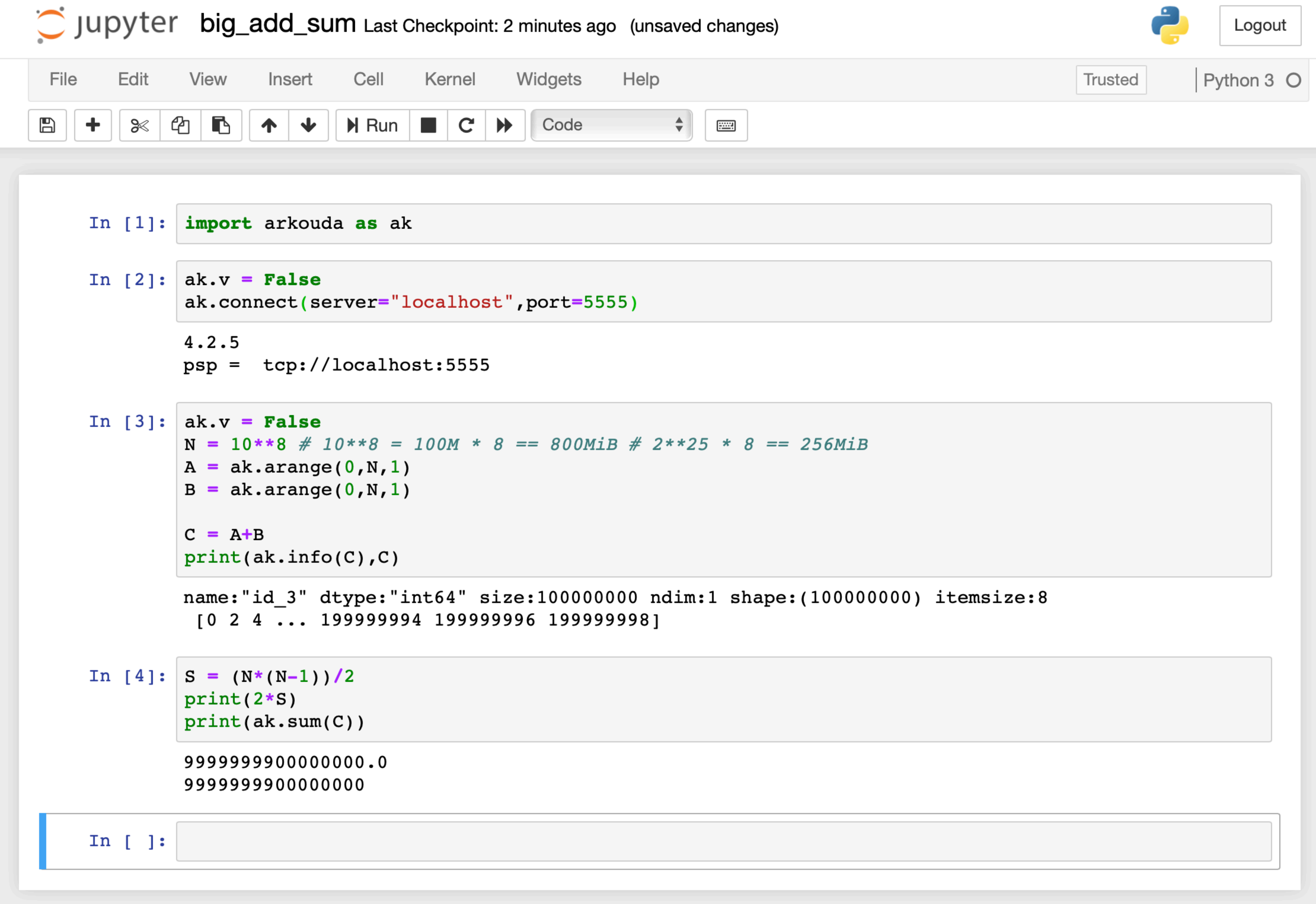
Chapel-Based Server

Massive
Flame Front
Supercomputer
…For…
Well Funded
Discriminating
Zelots
…or any other
computer even your
laptop

Why Chapel?

- High level — makes for less code
- Close to “Pythonic” (for a statically type language)
- Great support for array operations and distributed arrays
- Direct support for sync/atomic variables
- Same code runs on single or multi-locale — laptop to supercomputer

Screenshot 1



In [1]:

```
import arkouda as ak
```

In [2]:

```
ak.v = False
ak.connect(server="localhost",port=5555)
```

```
4.2.5
psp =  tcp://localhost:5555
```

In [3]:

```
ak.v = False
N = 10**8 # 10**8 = 100M * 8 == 800MiB # 2**25 * 8 == 256MiB
A = ak.arange(0,N,1)
B = ak.arange(0,N,1)

C = A+B
print(ak.info(C),C)
```

```
name:"id_3" dtype:"int64" size:100000000 ndim:1 shape:(100000000) itemsize:8
 [0 2 4 ... 199999994 199999996 199999998]
```

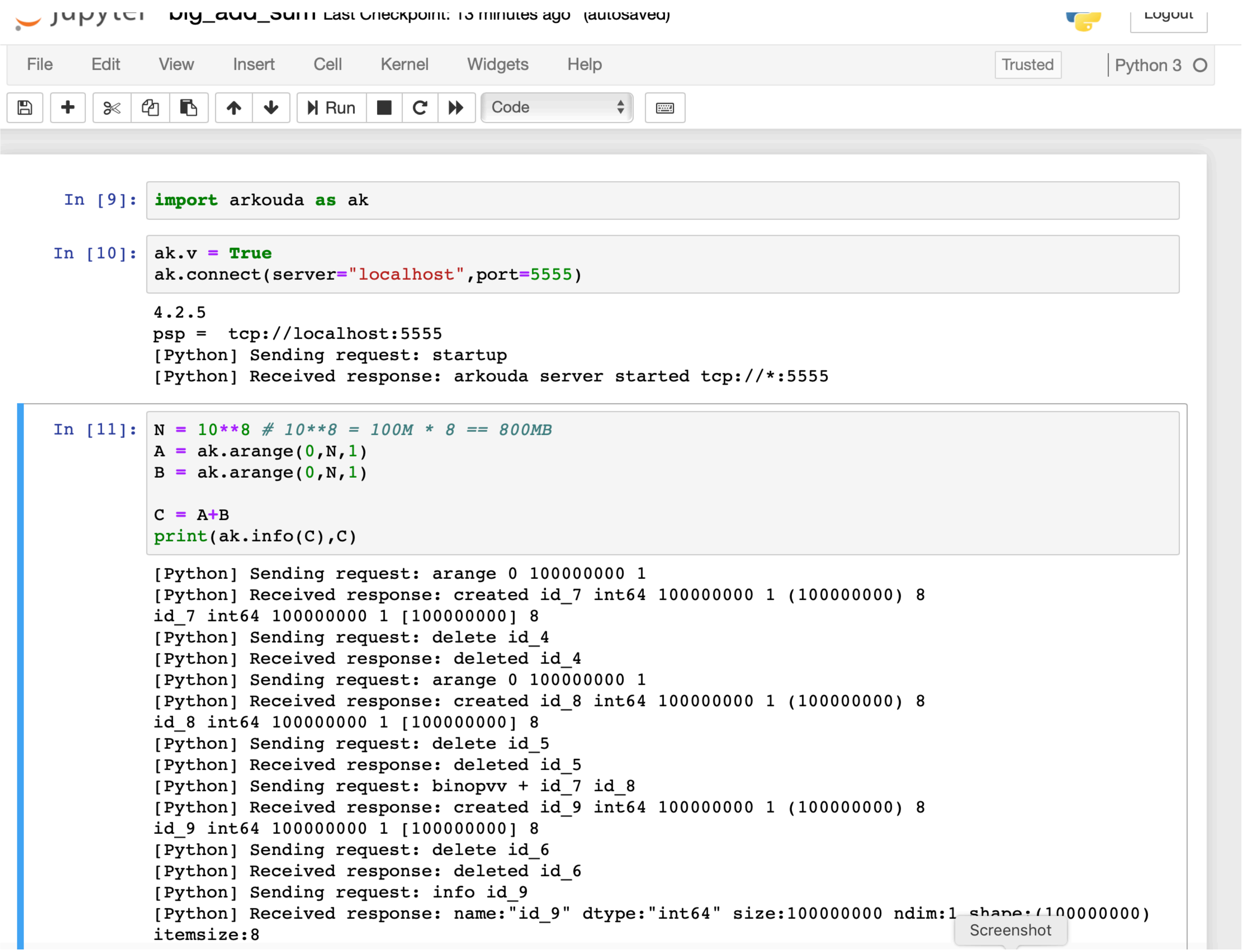
In [4]:

```
S = (N*(N-1))/2
print(2*S)
print(ak.sum(C))
```

```
9999999900000000.0
9999999900000000
```

In [ ]:

Screenshot 2



In [9]:
```
import arkouda as ak
```

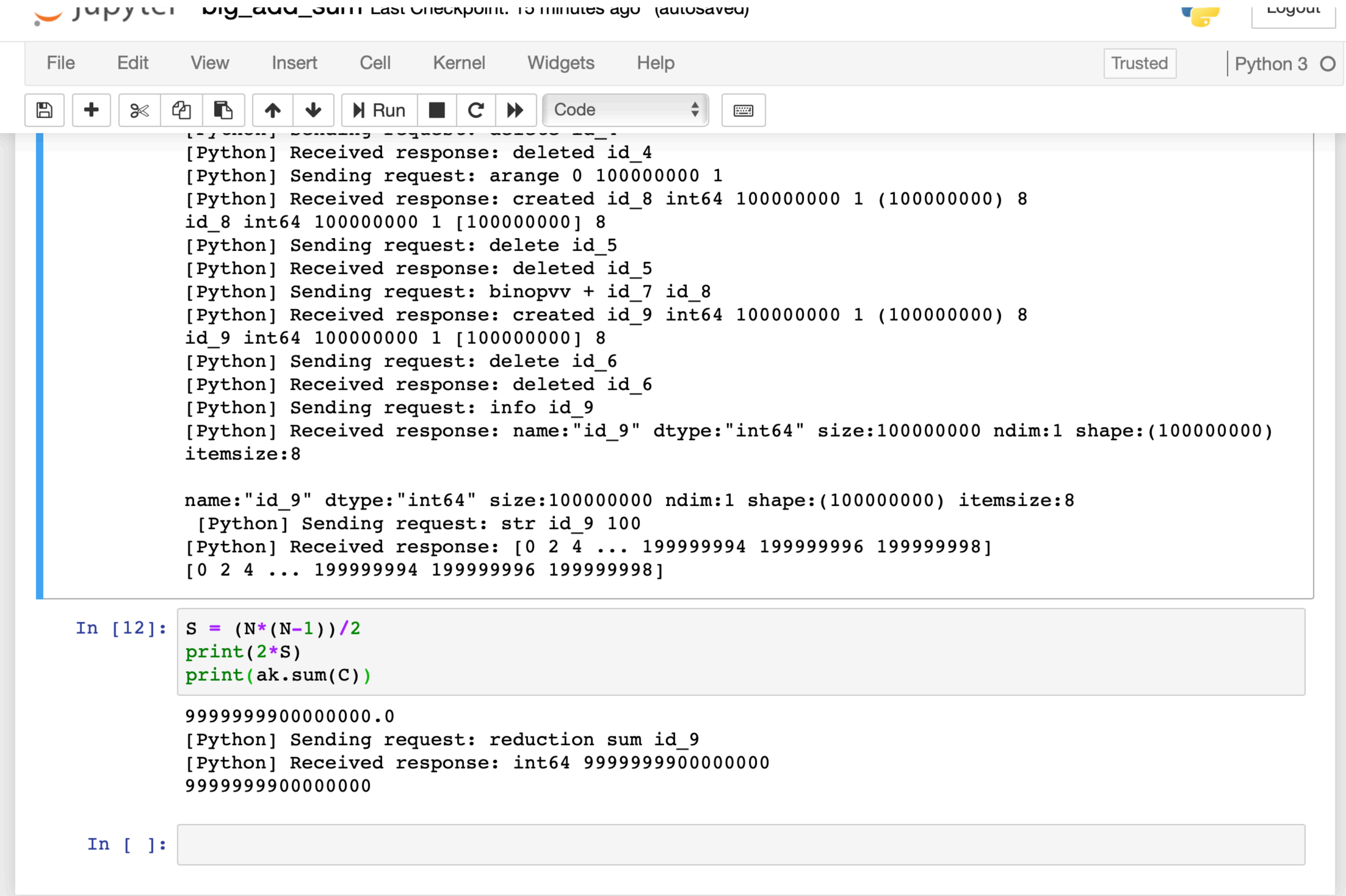
In [10]:
```
ak.v = True
ak.connect(server="localhost",port=5555)
```

```
4.2.5
psp =  tcp://localhost:5555
[Python] Sending request: startup
[Python] Received response: arkouda server started tcp://*:5555
```

In [11]:
```
N = 10**8 # 10**8 = 100M * 8 == 800MB
A = ak.arange(0,N,1)
B = ak.arange(0,N,1)

C = A+B
print(ak.info(C),C)
```

```
[Python] Sending request: arange 0 100000000 1
[Python] Received response: created id_7 int64 100000000 1 (100000000) 8
id_7 int64 100000000 1 [100000000] 8
[Python] Sending request: delete id_4
[Python] Received response: deleted id_4
[Python] Sending request: arange 0 100000000 1
[Python] Received response: created id_8 int64 100000000 1 (100000000) 8
id_8 int64 100000000 1 [100000000] 8
[Python] Sending request: delete id_5
[Python] Received response: deleted id_5
[Python] Sending request: binopvv + id_7 id_8
[Python] Received response: created id_9 int64 100000000 1 (100000000) 8
id_9 int64 100000000 1 [100000000] 8
[Python] Sending request: delete id_6
[Python] Received response: deleted id_6
[Python] Sending request: info id_9
[Python] Received response: name:"id_9" dtype:"int64" size:100000000 ndim:1 shape:(100000000)
itemsize:8
```

Screenshot 3



```
[Python] Sending request: delete id_4
[Python] Received response: deleted id_4
[Python] Sending request: arange 0 100000000 1
[Python] Received response: created id_8 int64 100000000 1 (100000000) 8
id_8 int64 100000000 1 [100000000] 8
[Python] Sending request: delete id_5
[Python] Received response: deleted id_5
[Python] Sending request: binopvv + id_7 id_8
[Python] Received response: created id_9 int64 100000000 1 (100000000) 8
id_9 int64 100000000 1 [100000000] 8
[Python] Sending request: delete id_6
[Python] Received response: deleted id_6
[Python] Sending request: info id_9
[Python] Received response: name:"id_9" dtype:"int64" size:100000000 ndim:1 shape:(100000000)
itemsize:8

name:"id_9" dtype:"int64" size:100000000 ndim:1 shape:(100000000) itemsize:8
 [Python] Sending request: str id_9 100
[Python] Received response: [0 2 4 ... 199999994 199999996 199999998]
[0 2 4 ... 199999994 199999996 199999998]
```

```
In [12]: S = (N*(N-1))/2
         print(2*S)
         print(ak.sum(C))
```

```
9999999900000000.0
[Python] Sending request: reduction sum id_9
[Python] Received response: int64 9999999900000000
9999999900000000
```

```
In [ ]:
```

Chapel Implementation Details

- I could make a whole talk about this…
- Implementing the array operations is straight forward in Chapel.
- Implementing function, operator, and type selection is where most of the code is in the implementation. This is an issue for all statically type languages.
- Flat multi-type symbol table…
    - Enum to mirror dtypes/types used, testable at runtime.
    - Chapel dynamic casts were important.
- Select constructs everywhere… moving to vtable like approach indexed by dtype/type enum.

Chapel Implementation Details

- Needed generic fields when using BlockDist arrays in a class
- Using PrivateDist for some optimizations
- Type-based nested procedures
- Need more meta programming facilities like macros or a way to auto generate from a template.
- Need a Chapel type primer/tutorial to show how to explicitly state a type… suggesting init() variants is sometimes not helpful.

Python Implementation Details

- We rely on Python’s scoping, reference counting, and GC.

- GC issue — Jupyter prevents garbage collection when you put a var in a cell to get the repr… the Out[] in Jupyter creates a reference to the object.

- Importing NumPy and using types and other features to extend functionality

- Pdarray object is a shim with a handle(name) of the array object in the Arkouda server

HDF5 Array I/O

- Currently the data we operate on comes in CSV files
- We use a Python Pandas/HDF5 process to convert CSV files into HDF5 files
- pip3 install hdflow
- Arkouda only has HDF5 I/O at the moment

A point of integration for HPC libraries and Python3

- Parallel Libraries:
  - FFT
  - Tensor
  - Graphs
  - Solvers
  - CHGL — Chapel Hyper Graph Library
  - Many others
- Anything you could link into a Chapel application and interface with…

Future Possibilities

- Better Fileset/Dataset I/O
- More NumPy/SciPy/Pandas functionality
- Linking in parallel libraries to make them available
- Persisted and shared workspaces
- Multiuser
- Maybe even send and interpret ASTs from Python3
- Julia?
- Sharing… open source - approved, just waiting on OGC licensing opinion

Conclusions

- Enable your data scientists to do larger scale analyses.
- Look at more data and gain insights from the experience.
- It was not that hard and a lot of goodness from several months of work.
- You could use this pattern for other useful things.