Data Science Needs Interactive Supercomputing

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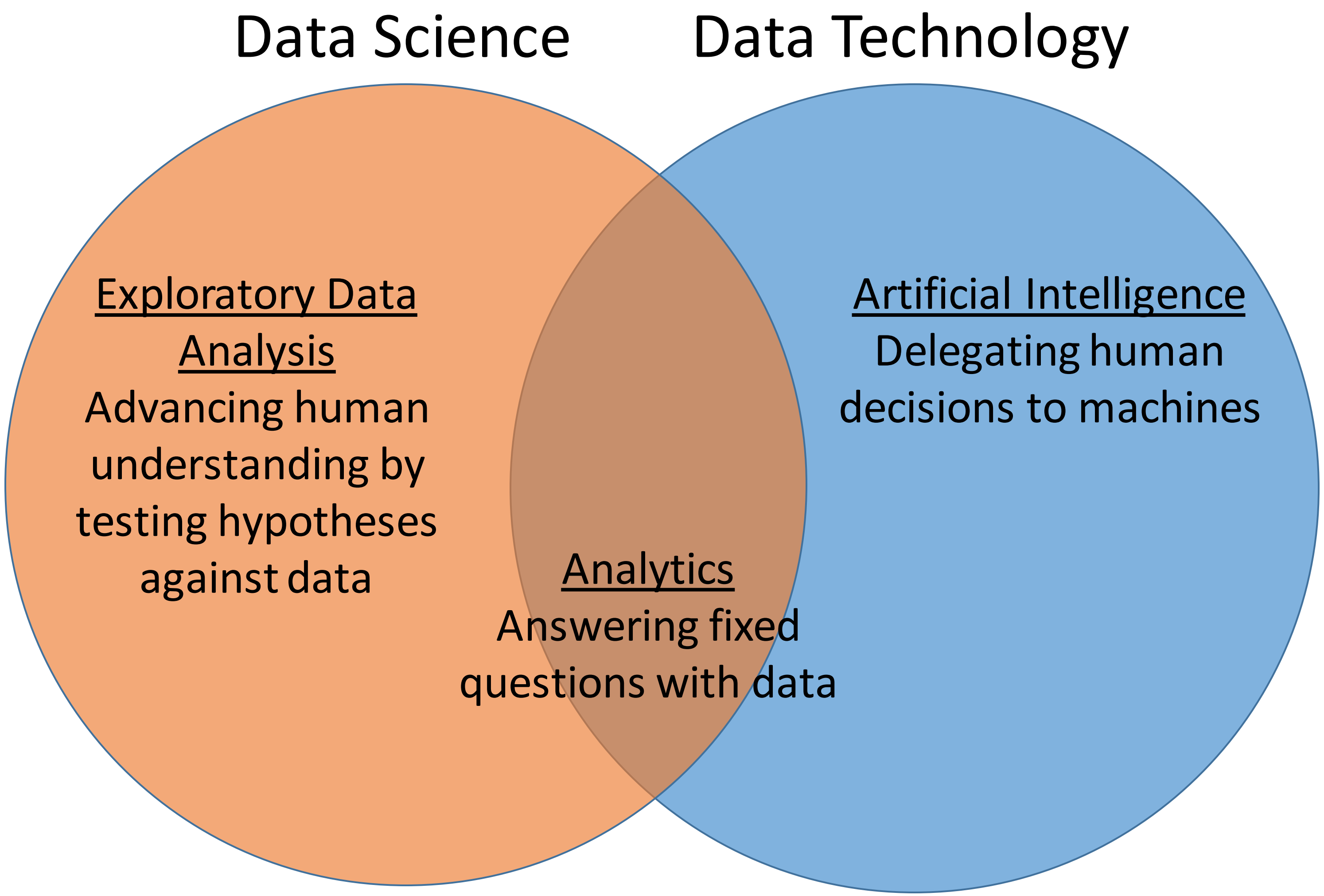
Why Data *Science*?

- Science: advancing human understanding of systems by building models tested against observation
- In most sciences, models are coupled to understanding

  Better understanding → more accurate model → more useful technology
- Data makes accurate* models possible without human understanding
- So why not skip to Data Technology?

“Can” Does Not Imply “Should”



Science is critical:

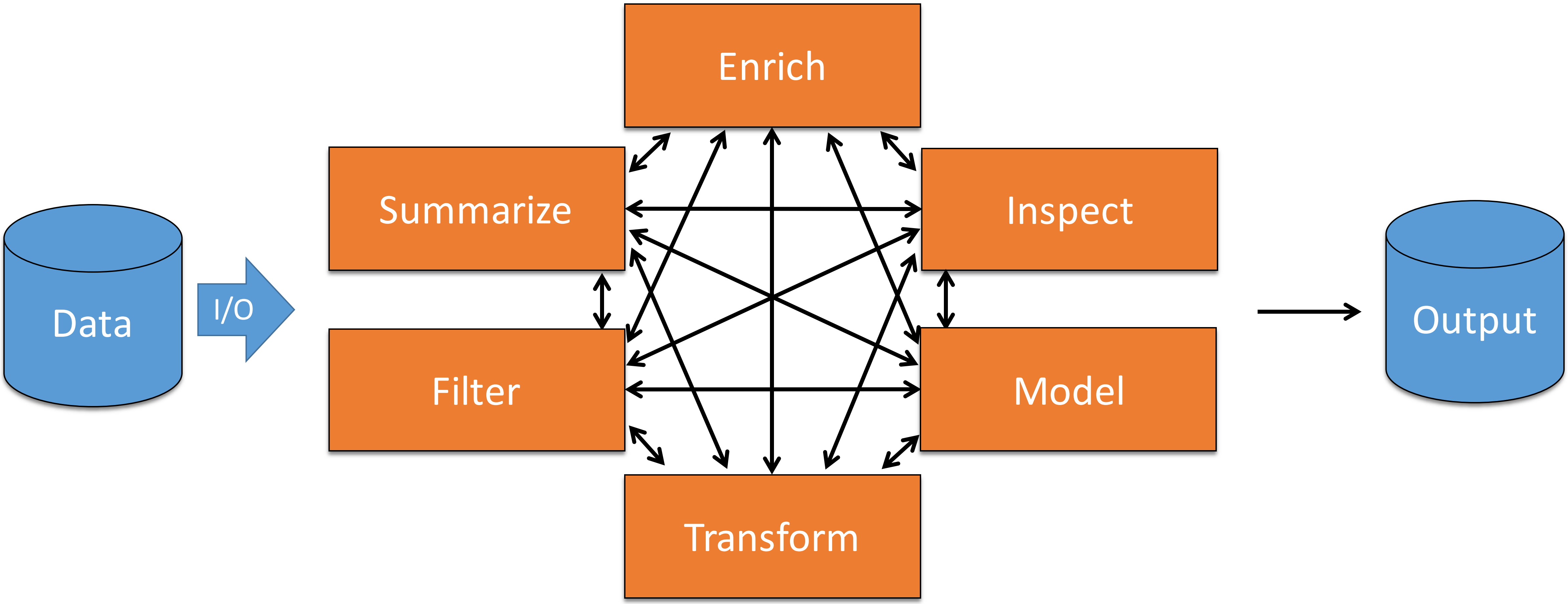
- Technology is not always the right goal
- Tech. without science will fail

And yet…

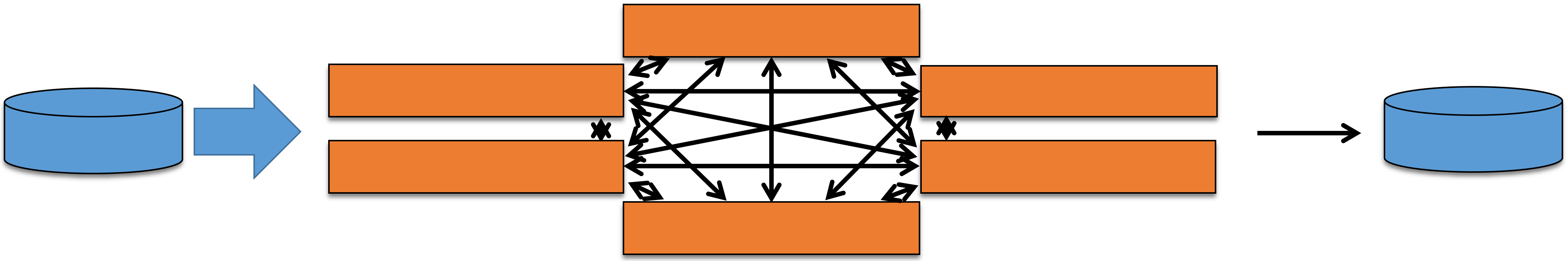
- Technology is what everyone talks about
- Large-scale tools favor tech. over science

(Data) Science is Interactive

"Hypothesis Testing"



Implications for Computing



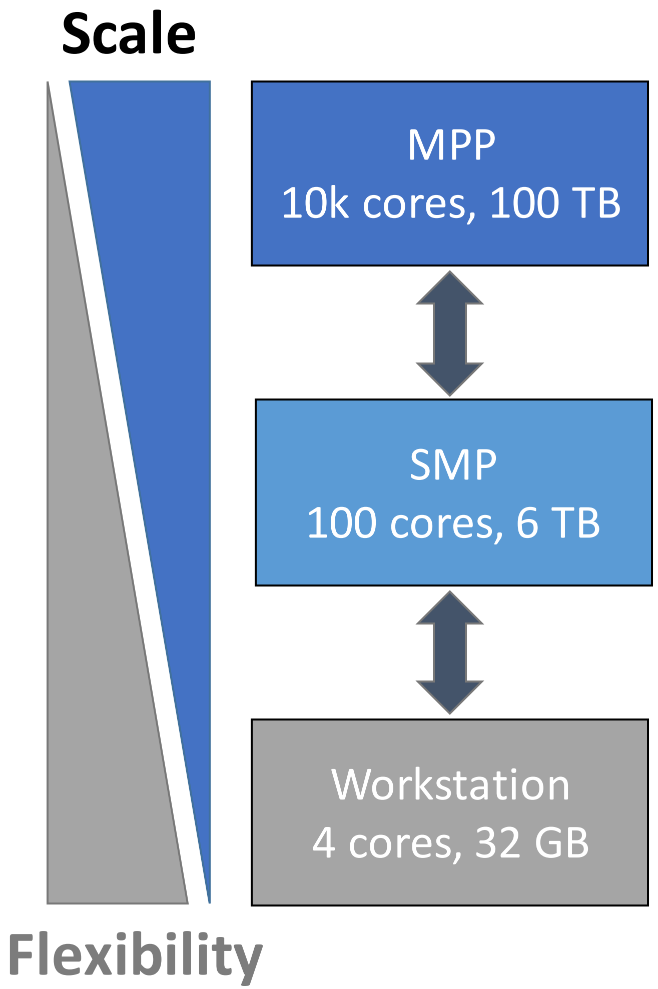
- Stay in memory
- Compute in small, reversible steps
- Enable introspection (code and state)
- Use other people's code
- Avoid boilerplate
- Maximize $\frac{t_{thinking}}{t_{thinking}+t_{coding}+t_{waiting}}$

So, basically Python…

…but fast

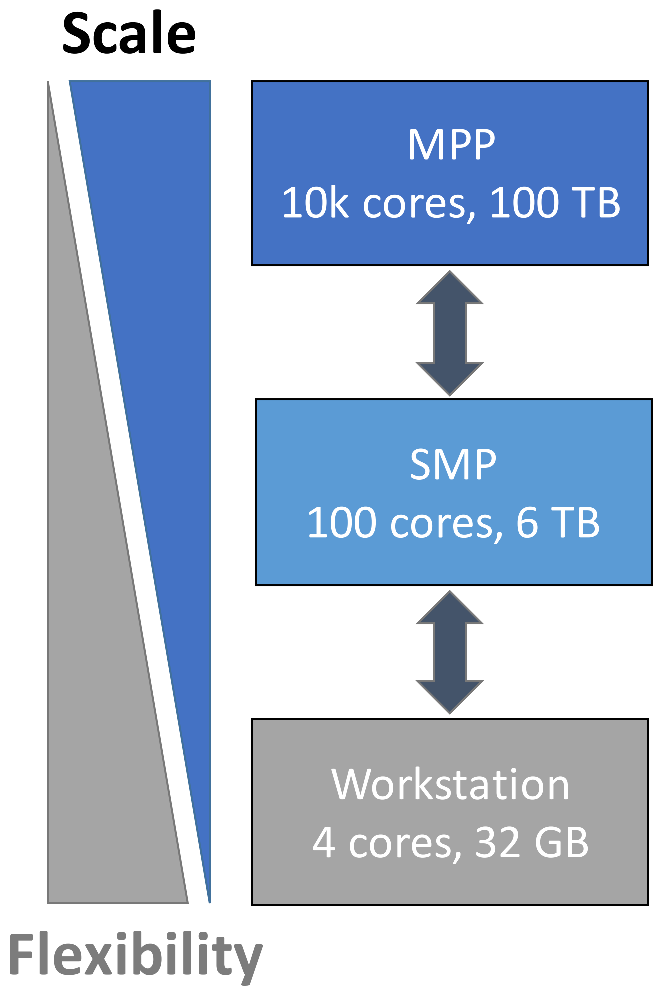
Interactive Computational Ladder

- Goal: Move seamlessly between tiers
  - Same data formats
  - Same UI (Jupyter)
  - Same APIs (NumPy/Pandas)
- Lower two tiers are easy



Interactive Computational Ladder

- We need the upper tier
  - Cybersecurity data >> 6 TB
- But hardware is the easy part
  - Need serious data engineering
  - Need to rethink job scheduling
  - Need an **HPC shell**



An HPC Shell for Data Science

Load Terabytes of data…

… into a familiar, interactive UI …

… where standard data science operations …

… execute within the human thought loop …

… and interoperate with optimized libraries.

Arkouda

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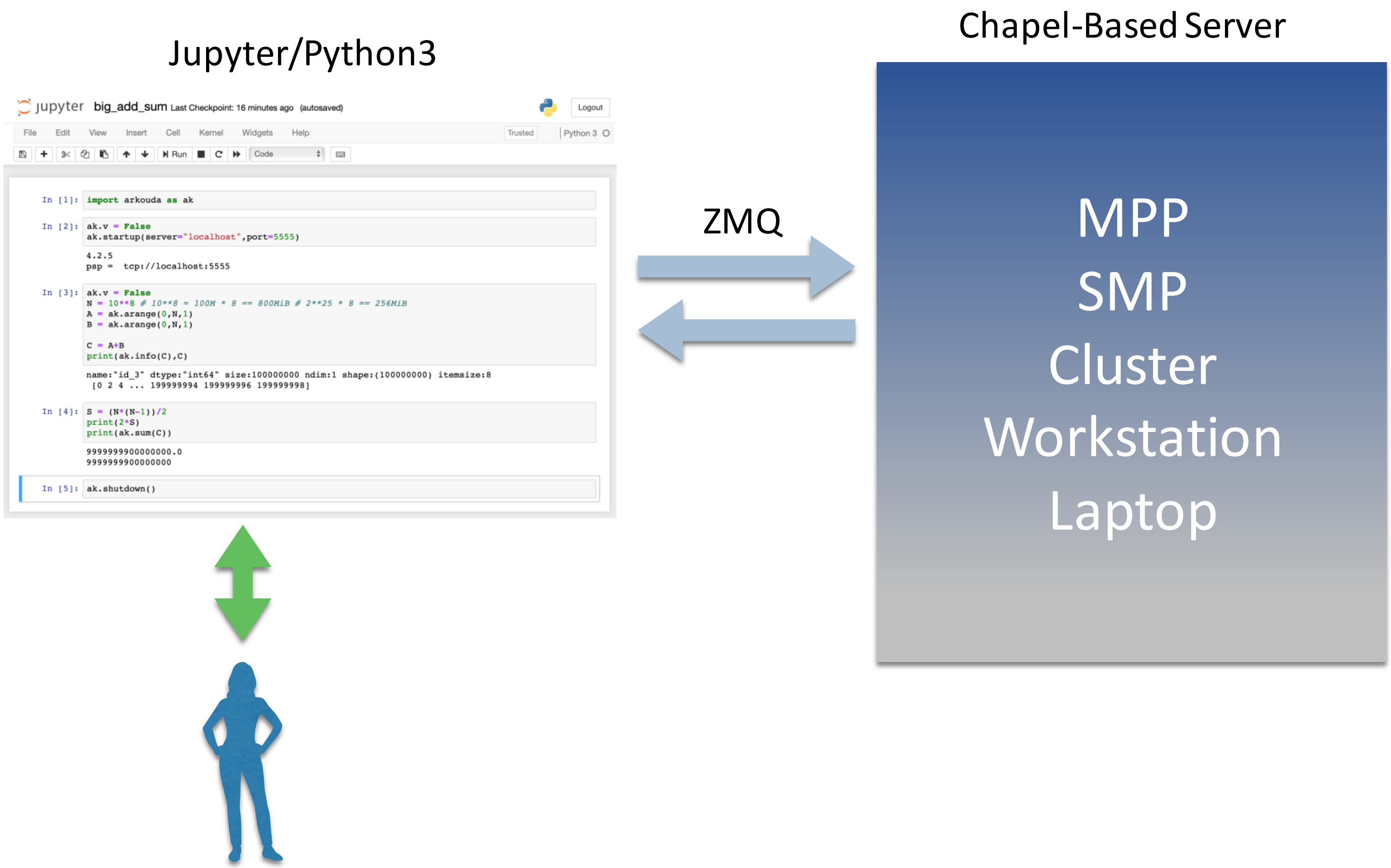
Arkouda: an HPC shell for data science

- Chapel backend (server)
- Jupyter/Python frontend (client)
- NumPy-like API

Arkouda Design



Arkouda Design

- Why Chapel?
  - High-level language with C-comparable performance
  - Parallelism is a first-class citizen
  - Great distributed array support
  - Portable code: from laptop up to supercomputer

Where Does Arkouda Fit In?

- Unique approach
  - Other efforts: interactivity → parallel, distributed execution
  - Arkouda: proven HPC performance → interactivity
- Arkouda uses the HPC
  - Scales positively to at least 10k cores
  - Exploits features of high-speed interconnects
  - Leverages parallel filesystems
  - **All without user fine-tuning**
- Current drawbacks
  - Still adding major features
  - Only one I/O format (HDF5)
  - No GPU support

Arkouda Startup

1) In terminal:

```
> arkouda_server -nl 96

server listening on hostname:port
```

2) In Jupyter:

```
In [2]: import arkouda as ak
        ak.connect(hostname, port)

4.2.5
psp =  tcp://nid00104:5555
connected to tcp://nid00104:5555
```

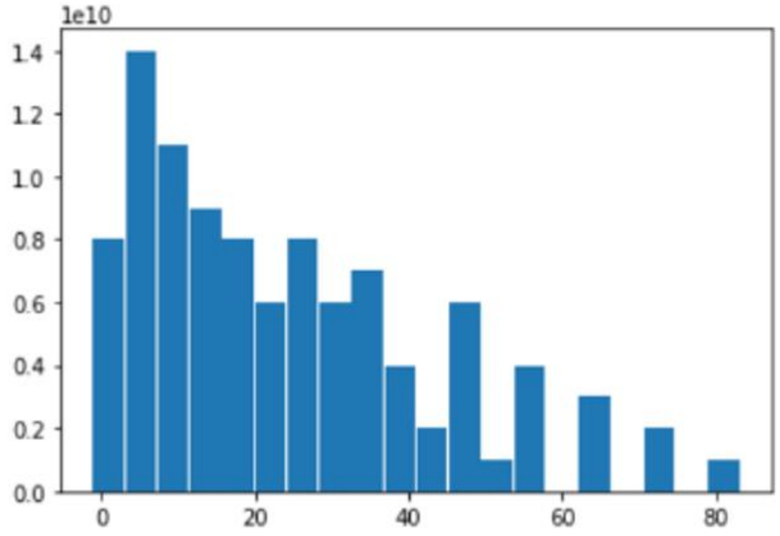
Data Exploration with Arkouda and NumPy

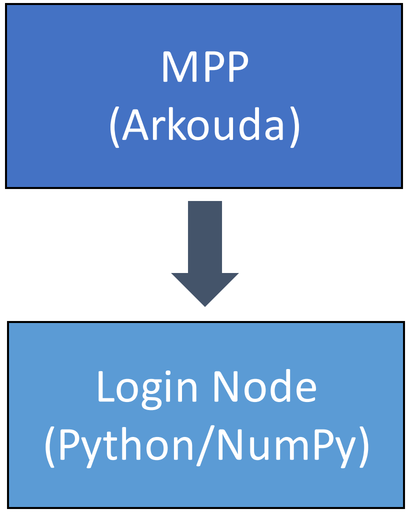
```
In [9]: A = ak.randint(0, 10, 10**11)
        B = ak.randint(0, 10, 10**11)
        C = A * B
        hist = ak.histogram(C, 20)
        Cmax = C.max()
        Cmin = C.min()
```

executed in 3.96s, finished 13:45:28 2019-09-12

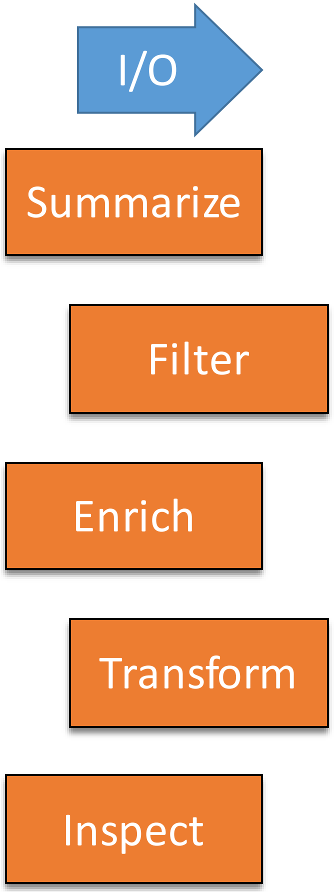
```
In [10]: bins = np.linspace(Cmin, Cmax, 20)
         _ = plt.bar(bins, hist.to_ndarray(), width=(Cmax-Cmin)/20)
```

executed in 193ms, finished 13:45:28 2019-09-12





Hypothesis Testing on 50 Billion Records



Operation	Example	Approximate Time (seconds)
Read from disk	A = ak.read_hdf()	30-60
Scalar Reduction	A.sum()	< 1
Histogram	ak.histogram(A)	< 1
Vector Ops	A + B, A == B, A & B	< 1
Logical Indexing	A[A == val]	1 - 10
Set Membership	ak.in1d(A, set)	1
Gather	B = Table[A]	30 - 300
Group by Key	G = ak.GroupBy(A)	60
Aggregate per Key	G.aggregate(B, 'sum')	15
Get Item	print(A[42])	< 1
Export to NumPy	A[:10**6].to_ndarray()	2

- A, B are 50 billion-element arrays
- Timings measured on real data
- Hardware: Cray XC40
  - 96 nodes
  - 3072 cores
  - 24 TB
  - Lustre filesystem

What about Model ?

- Vision: Expose HPC libraries to Python via Arkouda
  - FFT
  - Tensor decomposition
  - Graph algorithms
  - Solvers
  - CHGL (Chapel HyperGraph Library from PNNL)
  - Anything you could link into a Chapel application (via C or LLVM)
- Need to standardize a distributed array interface with the HPC community

Python Implementation Details

- Python pdarray class: a shim for the distributed array on the Arkouda server
  - Stores server-side name of array
  - Has a NumPy-like dtype
  - Has methods that translate operators into server commands
- Arkouda relies on Python to reduce complexity
  - Scoping
  - Reference counting
  - Garbage collection
  - Exceptions
- Arkouda integrates with and uses NumPy
  - Dtypes
  - Argument validation
  - Type conversion

Chapel Implementation Details

- A restricted Chapel interpreter:
  - Symbol table holding multi-type array wrappers
  - Code to parse commands from Python and select functions, operators, and types
- Chapel does some things really well
  - Makes parallelism easy (often implicit!)
  - Abstracts away inter-node communication and data layout
  - Compiler templates some functions
  - Allows dynamic casts from generic arrays to typed arrays
- But some things are hard
  - Large "select" statements for choosing functions, operators, types (an issue for all statically-typed languages)
  - Long compile times
- Far too many details to cover here…

Future Directions

- Open source release
- Tactical functionality
  - Strings and/or categorical dtype
  - Actual DataFrame class
  - Segmented arrays for sparse linear algebra (e.g. GraphBLAS)
- Strategic goals
  - Integration of Parallel Libraries
  - Multi-user support

Conclusion

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It’s not crazy.

Acknowledgements

- Michael Merrill – inventor and lead developer
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