Arkouda:
Terascale Data Science at Interactive Rates

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SciPy 2020

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chapel-lang.org
@ChapelLanguage
Motivation for Arkouda

**Motivation:** Say you’ve got…

...a bunch of Python programmers

...HPC-scale problems to solve

...access to HPC systems

How will you leverage your Python programmers to get your work done?

https://www.cscs.ch/computers/piz-daint/
Arkouda Design

**Python3 Client**

- ZMQ Socket

**Chapel Server**

- Dispatcher
  - Indexing
  - Arithmetic
  - Sorting
  - Generation
  - I/O

- Code Modules

- Distributed Array

- Meta

- Distributed Object Store

- Platform
  - MPP, SMP, Cluster, Laptop, etc.
## Data Science on 50 Billion Records

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<td>A.sum()</td>
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<td>Logical Indexing</td>
<td>A[B == val]</td>
<td>1 - 10</td>
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<tr>
<td>Set Membership</td>
<td>ak.in1d(A, set)</td>
<td>1</td>
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<td>Gather</td>
<td>B = Table[A]</td>
<td>4 - 120</td>
</tr>
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<td>Get Item</td>
<td>print(A[42])</td>
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<td>I = ak.argsort(A)</td>
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- A, B are 50 billion-element arrays of 32-bit values
- Timings measured on real data
- Hardware: Cray XC40
  - 96 nodes
  - 3072 cores
  - 24 TB
  - Lustre filesystem

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Presented at CHIUW 2020, May 22, 2019
Data Science Demands Interactivity

- Productivity with just enough performance
  - No compilation
  - No intermediate I/O
  - No writing boilerplate code
  - *Fast enough* to stay within thought loop

- Interactive Python on a large server satisfies these criteria for datasets up to 10-100 GB

presented at CHIUW 2020, May 22, 2019
Python Is Not Really Python

and many more Python packages

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Data Science Demands Scaling

- Must use the whole dataset
  - Unbiased sampling of large datasets is difficult
  - Even unbiased sampling eliminates rare and high-order effects
  - Physics of most datasets are global, not local
- Datasets have outgrown (normal) computers
  - Server memory: ~ 1 TB
  - Many datasets > 10 TB

presented at CHIUW 2020, May 22, 2019
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: an HPC shell for data science
• Chapel backend (server)
• Jupyter/Python frontend (client)
• NumPy-like API

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Arkouda: NumPy for HPC

- Feature extraction
- Scalable DataFrames
- Parallel, Distributed Runtime
- Large (hyper)graphs
- GPU code?
- HPC libraries?

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What is Chapel?

**Chapel**: A modern parallel programming language

- portable & scalable
- open-source & collaborative

**Goals:**

- Support general parallel programming
- Make parallel programming at scale far more productive
Why Chapel?

• From the lead Arkouda developers:
  • High-level language with C-comparable performance
  • Parallelism is a first-class citizen
  • Portable code: from laptop up to supercomputer
  • Integrates with (distributed) numerical libraries (e.g., FFTW, FFTW-MPI)
  • Close to “Pythonic” (for a statically typed language)
    • Lowers the barrier for users to modify the backend implementation

```
var D = {1..1000, 1..1000} dmapped Block(...),
A: [D] real;
forall (i,j) in D do
  A[i,j] = i + (j - 0.5)/1000;
```
Arkouda Design

Python3 Client

Chapel Server

ZMQ Socket

Dispatcher

Code Modules

Indexing

Arithmetic

Sorting

Generation

I/O

Distributed Object Store

Distributed Array

Meta

Platform

MPP, SMP, Cluster, Laptop, etc.

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A Chapel Interpreter

1. Client message
   “binopvv + id_1 id_2”

2. Module dispatch
   binopvv + id_1 id_2

3. Argument lookup and result allocation
   id_1
   id_2
   id_3

4. Parallel execution
   id_1
   id_2
   id_3

5. Return message
   “created id_3”

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Using Arkouda: Startup

1) Initialize server in terminal

```
> arkouda_server -nl 96
server listening on hostname:port
```

2) Connect to server in Jupyter

```python
import arkouda as ak
ak.connect(hostname, port)
```

```
4.2.5
psp = tcp://nid00104:5555
connected to tcp://nid00104:5555
```
Using Arkouda: Workflow

```
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
```
Arkouda Accomplishments

By taking this approach, these users were able to:

• interact with a running Chapel program from Python within Jupyter
• run the same back-end program on…
  …a Mac laptop
  …an Infiniband cluster
  …an HPE Superdome X
  …a Cray XC
• compute on TB-sized arrays in seconds
• with 1-2 person-months of effort
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# NumPy vs. Arkouda Performance

Performance normalized to NumPy

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<th>NumPy</th>
<th>Arkouda (serial)</th>
<th>Arkouda (1-node/36-core)</th>
<th>Arkouda (512-node)</th>
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<tr>
<td>argsort</td>
<td>1.0</td>
<td>2.0</td>
<td>16.7</td>
<td>1837.3</td>
</tr>
<tr>
<td>coargsort</td>
<td>1.0</td>
<td>2.3</td>
<td>16.7</td>
<td>984.7</td>
</tr>
<tr>
<td>gather</td>
<td>1.0</td>
<td>0.4</td>
<td>11.7</td>
<td>469.1</td>
</tr>
<tr>
<td>reduce</td>
<td>1.0</td>
<td>1.2</td>
<td>12.0</td>
<td>4412.4</td>
</tr>
<tr>
<td>scan</td>
<td>1.0</td>
<td>0.8</td>
<td>3.2</td>
<td>266.6</td>
</tr>
<tr>
<td>scatter</td>
<td>1.0</td>
<td>1.0</td>
<td>11.8</td>
<td>781.8</td>
</tr>
<tr>
<td>stream</td>
<td>1.0</td>
<td>0.7</td>
<td>6.2</td>
<td>1590.4</td>
</tr>
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Cray XC (Aries network)
36-core (72 HT), 128 GB RAM
dual 18-core “Broadwell”, 2.1 GHz
Arkouda Scaling: **Aries at scale** (512 locales, 18k cores)

Sample result: Sorted 8TB of IPV4 addresses using 18k cores in just over a minute
Arkouda Scaling: Aries vs. IBV (32 locales, 1152 cores)
What about Dask?

- Arkouda performs significantly faster in our experience*
  - Comparison involves reading from HDF5 file and doing a scalar reduction
  - *Looking to work with Dask experts to ensure a fair comparison
- Dask configuration on HPC systems is not trivial
  - Getting Arkouda performance out the box is easy
- Dask is not designed for shuffle-based workflows (sorting, grouping, etc.)
  - Arkouda targets these workflows and scales without lazy evaluation
- Dask is much more established and featureful
  - Better integration with Pandas and more supported data formats
  - Excellent cluster management tooling
Arkouda Status

• Now 12,000+ lines of Chapel code, developed in one year
  • “without Chapel, we could not have gotten this far this fast”

• Open source:
  • Being developed on GitHub
  • Available as a PyPI package via ‘pip install arkouda’

• Being used on a daily / weekly basis on real data and problems
  • Features being added as requested by users
Arkouda Summary & Next Steps

• Arkouda is a powerful tool and vision
  • NumPy/Pandas on TB-scale arrays in seconds to minutes
  • A workbench for interactive HPC-scale data science
• Arkouda takes a unique approach to interactivity in HPC
  • Starts with performance and builds towards interactivity
• Next steps involve expanding API and supporting multi-user sessions
  • Actual dataframes (currently informal collections of arrays)
  • Sparse linear algebra (GraphBLAS)
  • Wrapping existing HPC libraries
  • Data sharing and access control
For More Information

- Arkouda GitHub: https://github.com/mhmerrill/arkouda
- Arkouda PyPi page: https://pypi.org/project/arkouda/
- Arkouda Gitter Channel: https://gitter.im/ArkoudaProject/community
- Bill Reus’s CHIUW talk: https://chapel-lang.org/CHIUW2020.html#keynote

- Chapel website: https://chapel-lang.org
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