Squeezing Performance out of Arkouda

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 @ChapelLanguage

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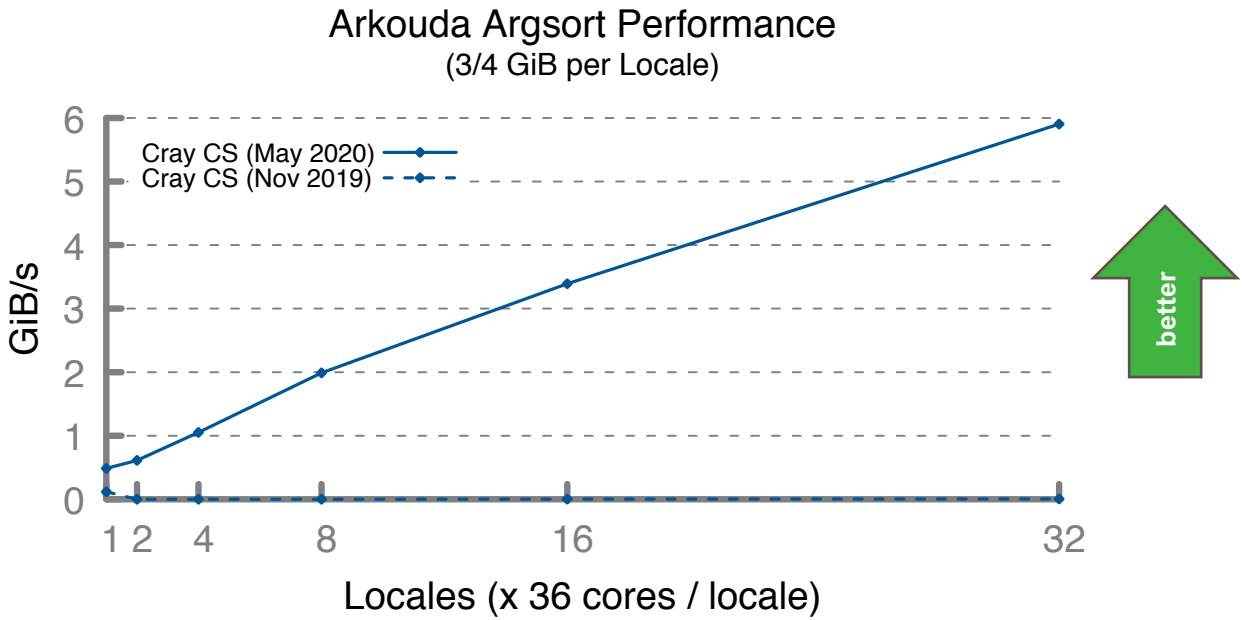
Teaser

- Achieved more than a 1000x speedup for sorting on InfiniBand systems



Testing Hardware

- Most performance results will be shown for Cray CS and Cray XC systems
  - 32-node Cray CS with 56 Gb/s InfiniBand network (1,152 cores)
  - 512-node Cray XC with Aries network (18,432 cores)
- Per-node hardware is similar for both systems
  - 36-core (72-thread) 2.1 GHz Broadwell processors
  - 128 GiB RAM
- Results for other networks will be shown at the end
  - Cray CS with 100 and 200 Gb/s InfiniBand networks
  - AWS clusters with 25 and 100 Gb/s Ethernet networks

Outline

- NumPy vs Arkouda Performance
- Sorting Background
- Small Message Performance
- Message Aggregation
- Aggregated Sort Performance
- Future work

Arkouda Background

- See Bill Reus's CHIUW 2020 keynote on Arkouda for details
- At a high level: Arkouda provides NumPy-like arrays at HPC scale
  - A NumPy/Pandas Python interface, backed by Chapel
  - Chapel provides performance and scalability

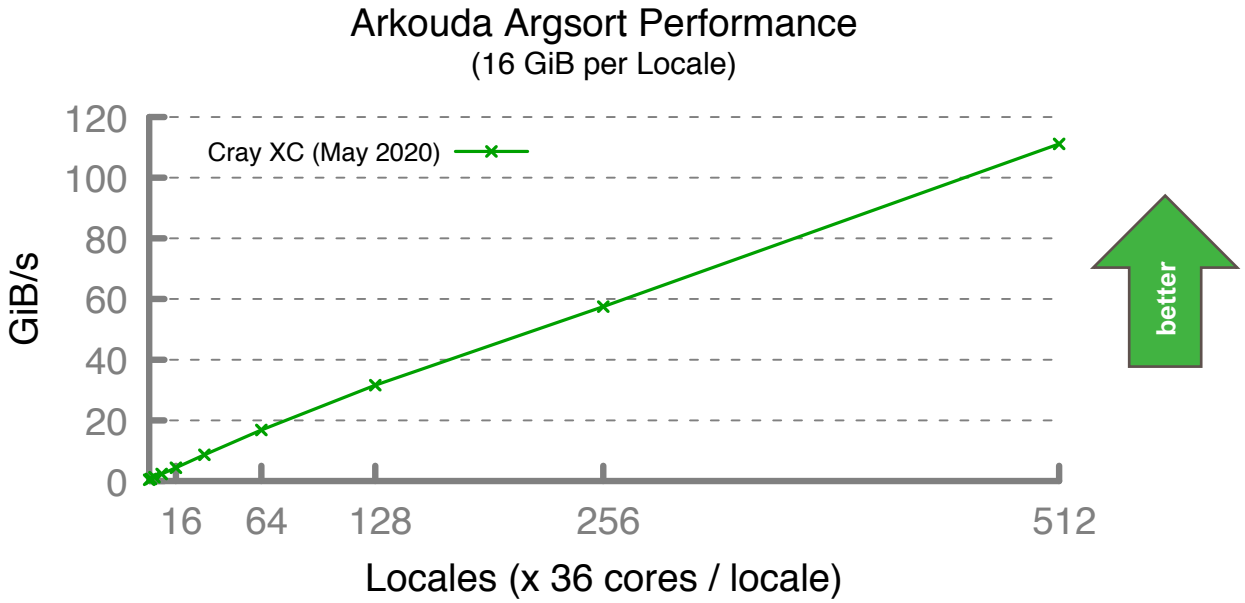
NumPy vs Arkouda Performance

- Performance normalized to NumPy on a Cray XC

benchmark	numpy	ak (serial)	ak (36-core)	ak (512-node)
argsort	1.0	2.0	16.7	1837.3
coargsort	1.0	2.3	16.7	984.7
gather	1.0	0.4	11.7	469.1
reduce	1.0	1.2	12.0	4412.4
scan	1.0	0.8	3.2	266.6
scatter	1.0	1.0	11.8	781.8
stream	1.0	0.7	6.2	1590.4

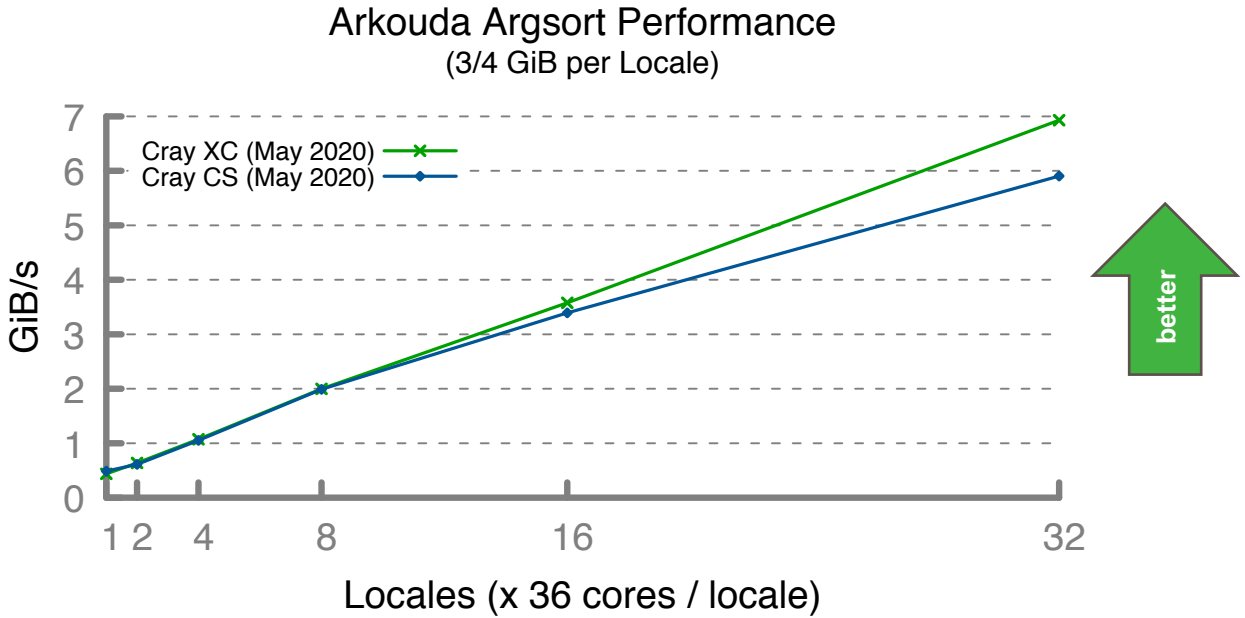
Current Argsort Performance

- Argsort has excellent performance and scalability on a Cray XC
  - 110 GiB/s at 512 nodes, sorting 8TiB of data in ~75 seconds



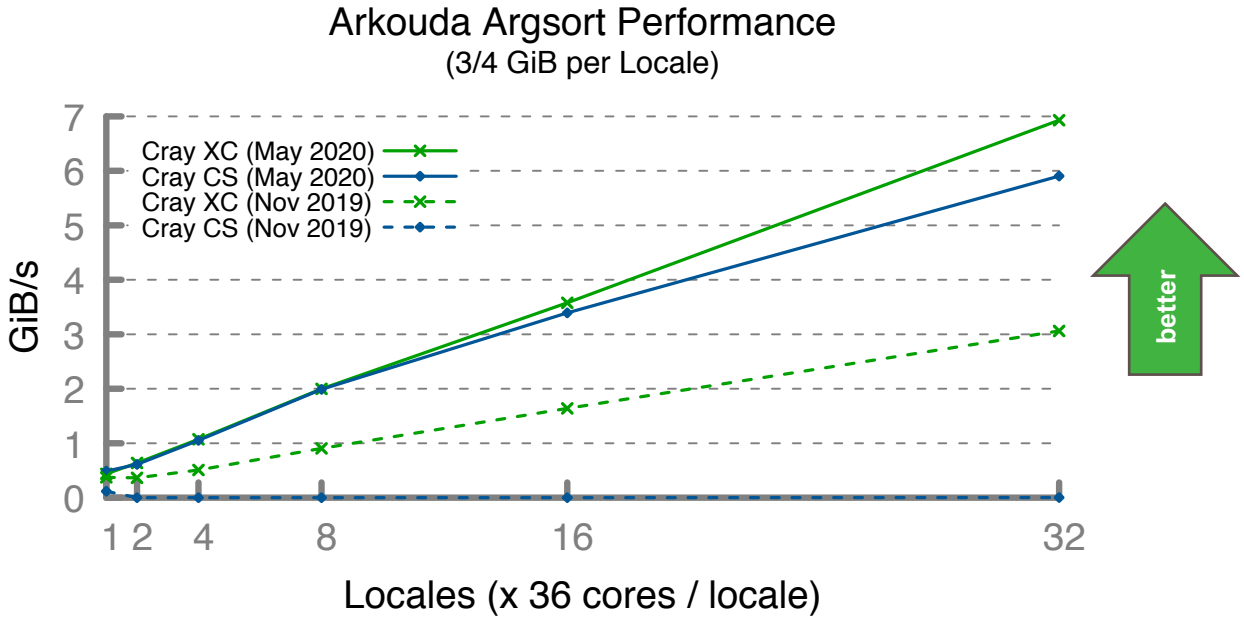
Current Argsort Performance

- Argsort performance is portable to InfiniBand networks
  - Similar performance up to 32 nodes



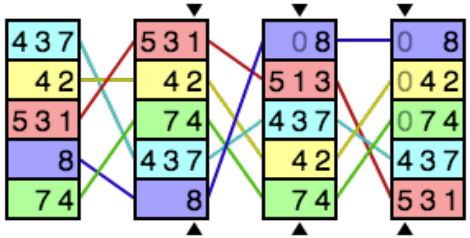
Original Argsort Performance

- Performance 6 months ago was a very different story
  - Respectable XC performance, unusable CS performance



Sorting Implementation

- Arkouda uses a simple 100 line least-significant-digit radix sort
  - Easy to parallelize, but lots of communication $O(wn)$
    - w is the number of digits (16-bit digits), n is the number of elements
    - 50B element array of 32-bit values has 100B 8-byte network transactions
  - Want to optimize without sacrificing maintainability and simplicity



https://www.growingwiththeweb.com/sorting/radix-sort-lsd/

Small Message Performance

- Previously, Arkouda used 'unorderedCopy()' for these 8-byte messages
  - Optimized copy for when no overlap will occur
- Sample performance for copying a 32 MiB local array to a remote array

```
// bulk
rArr = lArr;


// unordered
forall (r, l) in zip(rArr, lArr) do
  unorderedCopy(r, l);
```

Performance (MiB/s)		
config	**bulk**	**unordered**
Cray XC	8000.0	510.0
Cray CS	6000.0	2.0

Message Aggregation

- Added copy aggregators to Arkouda
  - Created for each task, must specify whether source or destination is remote

```
// bulk
rArr = lArr;


// unordered
forall (r, l) in zip(rArr, lArr) do
  unorderedCopy(r, l);


// aggregated
forall (r, l) in zip(rArr, lArr) with (var agg = new DstAggregator(int)) do
  agg.copy(r, l);
```

Performance (MiB/s)			
config	**bulk**	**unordered**	**aggregated**
Cray XC	8000.0	510.0	2275.0
Cray CS	6000.0	2.0	1850.0

Message Aggregation Implementation

```
config const bufferSize = 4096;


/*
 * Aggregates copy(ref dst, src). Optimized for when src is local.
 * Not parallel safe and is expected to be created on a per-task basis
 * High memory usage since there are per-destination buffers
 */
record DstAggregator {

  type elemType;
  var buffer: [LocaleSpace][0..#bufferSize] (addr, elemType);
  var bufferIdxs: [LocaleSpace] int;
```


Message Aggregation Implementation

```
inline proc copy(ref dst: elemType, srcVal: elemType) {
  // Get the locale of dst and the local address on that locale
  const loc = dst.locale.id;
  const dstAddr = getLocalAddr(dst);


  // Get our current index into the buffer for dst's locale
  ref bufferIdx = bufferIdxs[loc];


  // Buffer the address and desired value
  buffer[loc][bufferIdx] = (dstAddr, srcVal);
  bufferIdx += 1;


  // If full, flush
  if bufferIdx == bufferSize then
    flushBuffer(loc, bufferIdx);
}
```


Message Aggregation Implementation

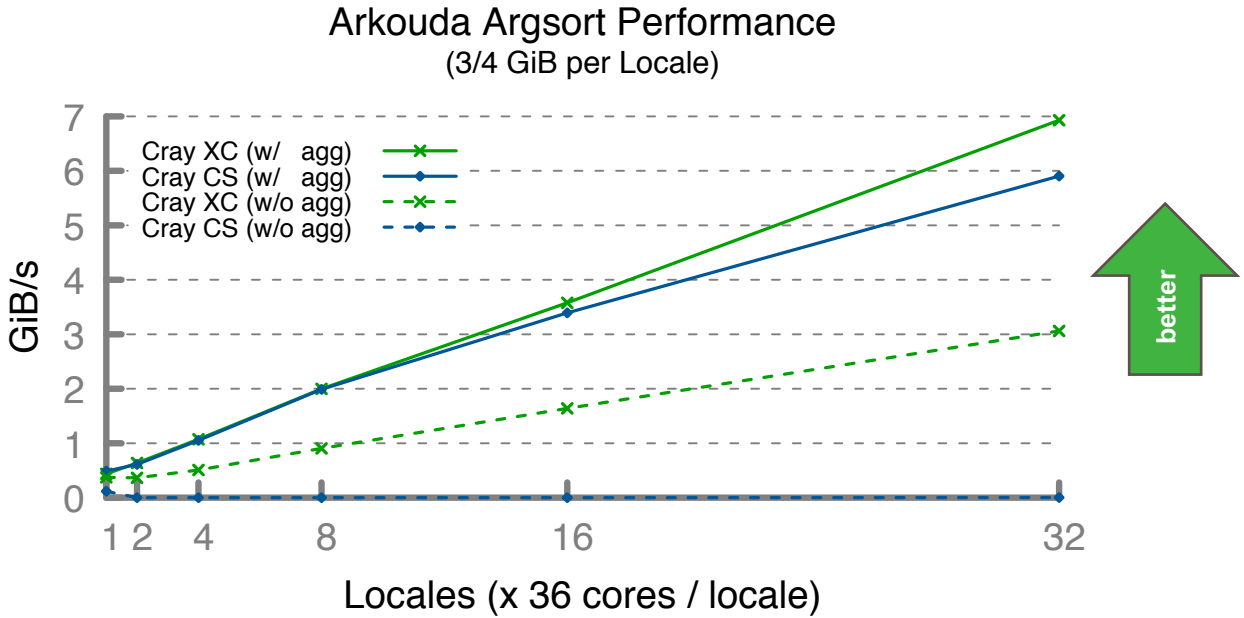
```
proc flushBuffer(loc: int, ref bufferIdx) {

  // Migrate execution to the remote node
  on Locales[loc] {
    // GET the buffered dst addrs and src values, and assign
    var localBuffer = buffer[loc][0..#bufferIdx];
    for (dstAddr, srcVal) in localBuffer do
      dstAddr.deref() = srcVal;
  }
  bufferIdx = 0;

}
```

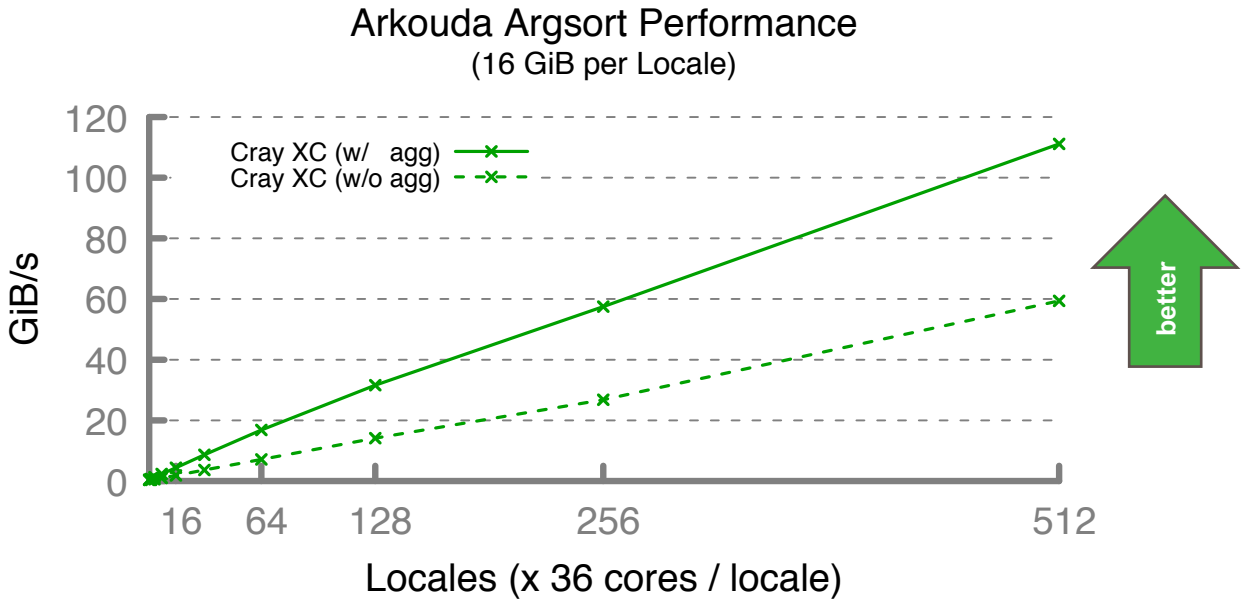

Aggregated Argsort Performance

- Aggregation improved performance by more than 2x on XC and 1000x on CS



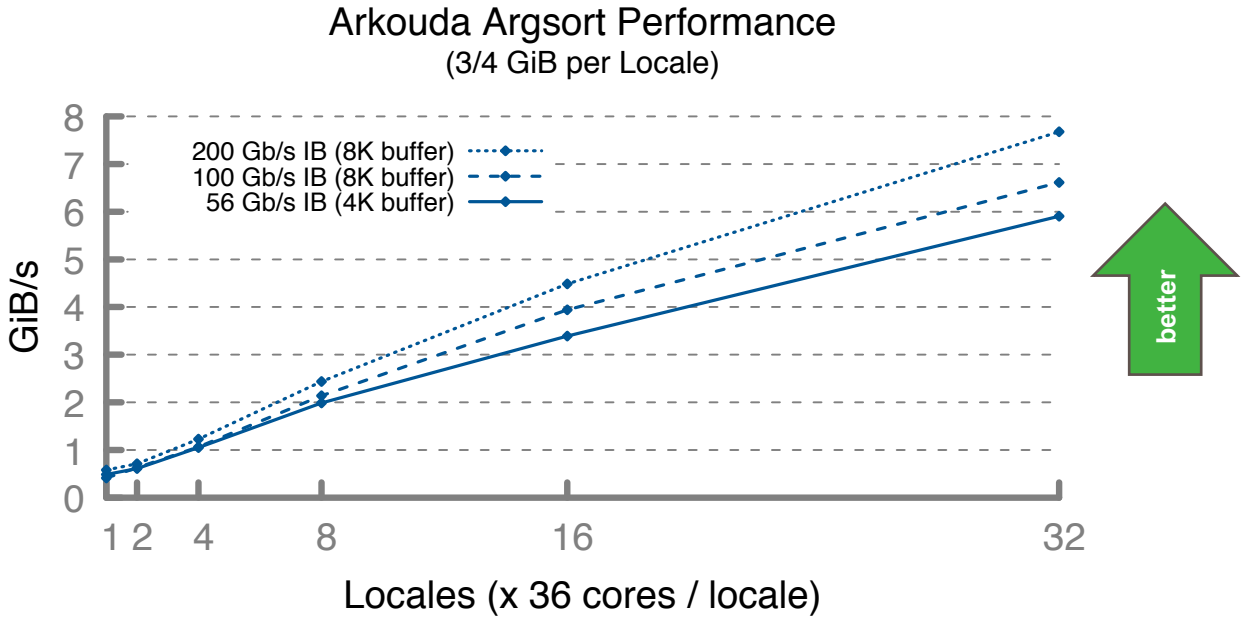
Aggregated Argsort Performance

- Aggregation has good scalability despite simple design



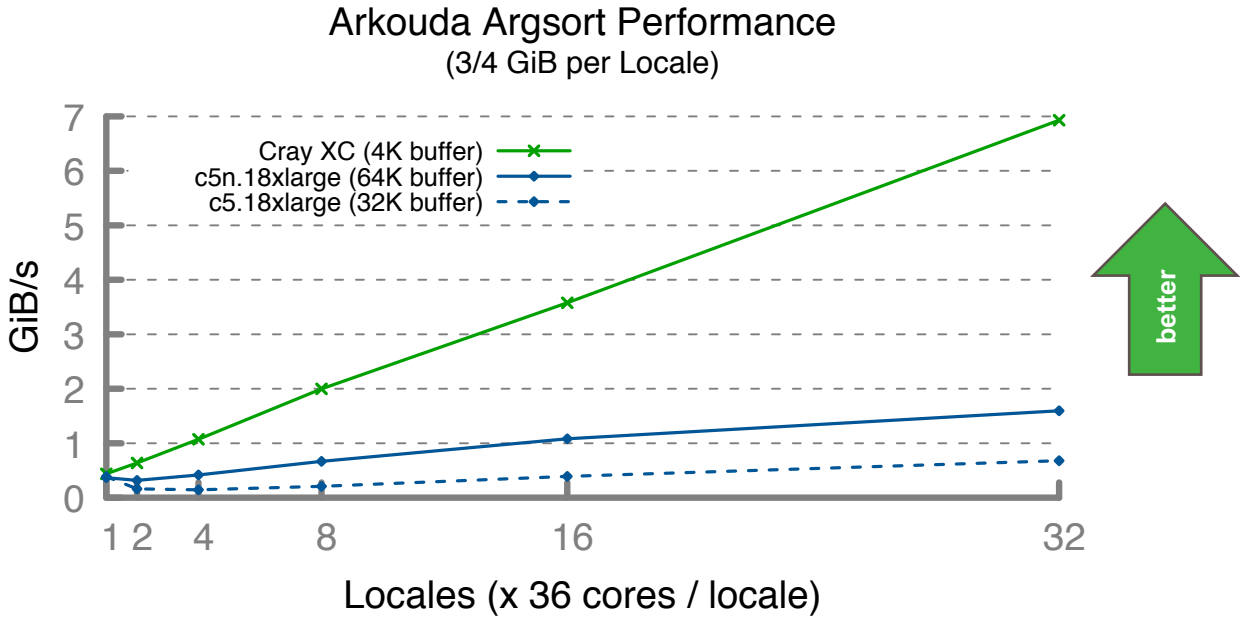
InfiniBand Performance

- Cray CS performance with 56, 100, and 200 Gb/s InfiniBand networks
  - Collected using 36-cores (200 Gb/s has 48 cores, but only 36 used)



Ethernet Performance

- AWS performance with 25 and 100 Gb/s Ethernet networks
  - Collected on 36-core c5.18xlarge and c5n.18xlarge w/ Elastic Fabric Adapter



More Information

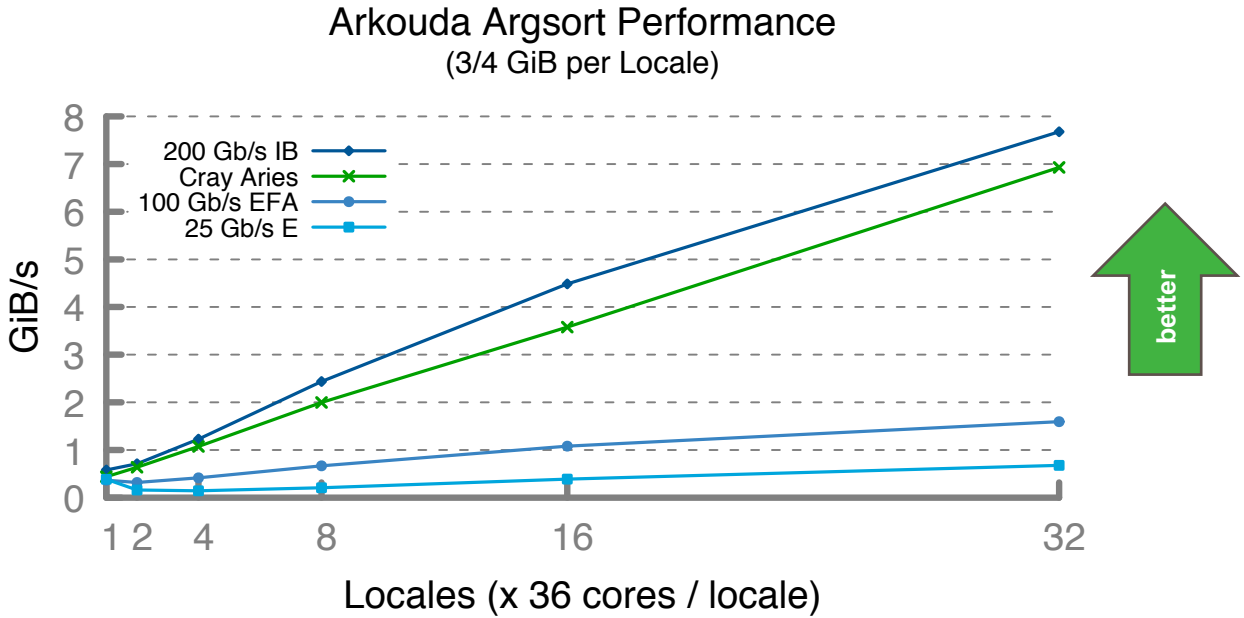
- For more information about other Arkouda optimizations see:
  - https://chapel-lang.org/releaseNotes/1.21/05-user-opt.pdf
- For more information about recent Chapel performance optimizations see:
  - https://chapel-lang.org/releaseNotes/1.21/04-perf-opt.pdf
- For general information about Chapel's performance and tuning tips see:
  - https://chapel-lang.org/performance.html

Future Work

- Collect Dask performance results
  - We have only anecdotal evidence that Arkouda is much faster
- Optimize aggregation performance and reduce memory footprint
  - Autotune buffer size on startup
  - Aggregate within a node before sending over the network
- Tune performance more for commodity networks and newer HPC networks
  - Ethernet and modern InfiniBand performance seem low
- Add aggregation to Chapel's standard library
  - Enable arbitrary message aggregation, not just copy aggregation

Summary

- Message aggregation enables a portable high performance sort in Arkouda
  - Significant performance optimization opportunities remain



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