User Application Optimizations

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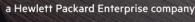


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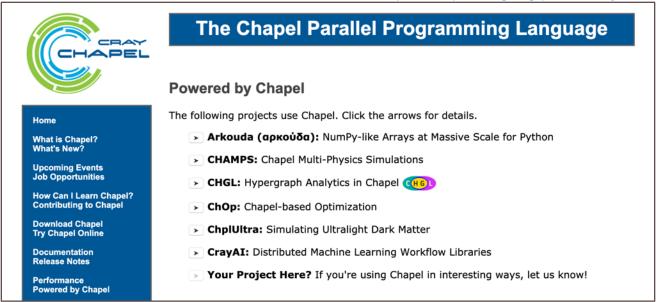


User Applications: Background



Chapel has seen an uptick in users with substantial applications

https://chapel-lang.org/poweredby.html



Has resulted in optimization/tuning collaborations with the Chapel team

Outline

- <u>DistributedFFT (from ChplUltra)</u>
- Arkouda



DistributedFFT (from ChplUltra)



DistributedFFT: Background

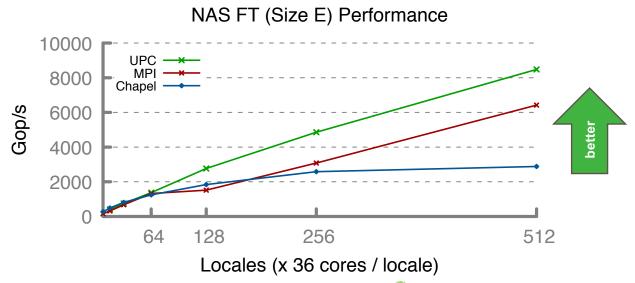


- DistributedFFT provides a distributed 3D FFT
 - https://github.com/npadmana/DistributedFFT
- Used as the foundation for an Ultralight Dark Matter (ULDM) Simulation
 - Originally used Python/pyFFTW, but problem size soon exceeded single node
 - Chapel was chosen for distributed nature and high performance
- Chapel port uses FFTW for serial FFT computations
 - Chapel is responsible for data distribution, parallelism, and communication
 - Showcases Chapel's interoperability features

DistributedFFT: Background



- Initial Chapel port provided significant performance improvements over Python
 - Added NAS-FT benchmark to validate and compare to traditional HPC
 - Performance was decent, though lagged UPC/MPI at 64 nodes or more



DistributedFFT: This Effort

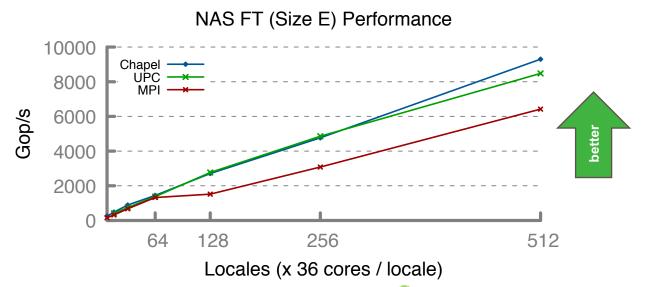


- Implemented several algorithmic optimizations
 - FFTW batching and plan caching, added comm/compute overlap
- Identified Chapel performance bottlenecks
 - Point-to-point array slice assignment has overhead
 - Only optimized for 'A = B', not 'A[locale0] = B[locale1]'
 - Local array assignment is not parallelized (uses serial 'memcpy')
- Opened Chapel issues for performance issues, worked around in the meantime
 - Using comm primitives (PUT/GET), manually parallelizing array assignment

DistributedFFT: Impact



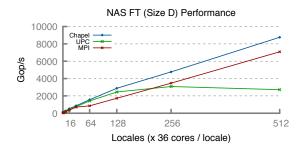
- Significantly improved performance and scalability (3x faster at 512 nodes)
 - Performance ahead of MPI
 - On par with highly optimized non-blocking UPC

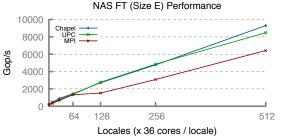


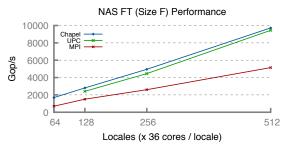
DistributedFFT: Impact



- Good performance across small, medium, and large problem sizes
 - Due to data decomposition, one-sided overlapping comm, FFTW batching







DistributedFFT: Next Steps



- Implement fixes for upstream Chapel performance issues
- Explore using cuFFT to offload FFT computations to GPUs

Arkouda



Arkouda: Background



- Arkouda provides NumPy-like arrays at HPC scale
 - A NumPy/Pandas Python interface, backed by Chapel
 - https://github.com/mhmerrill/arkouda
 - One of the largest open-source projects using Chapel
- Widespread adoption requires performing well on a wide variety of platforms
 - Has motivated several improvements to the Chapel compiler and runtime
- Some key operations use fine-grained communication (many 8-byte messages)
 - Cray Aries can achieve high rates for small messages
 - Other networks have much lower rates for small messages

Arkouda Aggregation: Background



- Previously, Arkouda used 'unorderedCopy()' for fine-grained messages
 - On Cray Aries, bulk copies achieve 8000 MB/s
 - unorderedCopy achieves 1000 MB/s (1/8 of bulk copy rate)
 - On 56 Gb FDR InfiniBand, bulk copies achieve 6000 MB/s
 - unorderedCopy only achieves 3 MB/s per node (1/2000 of bulk copy rate)
- In order to get performance on IB, small message aggregation is needed
 - Room for improvement on Aries as well

Arkouda Aggregation: This Effort



- Added copy aggregators to Arkouda
 - Aggregators must be created for each task
 - Have to specify type and whether source or destination is remote

```
forall i in D do
    unorderedCopy(revA[n-i], A[i]);
=>
forall i in D with (var agg = new DstAggregator(int)) do
    agg.copy(revA[n-i], A[i]);
```

Arkouda Aggregation: Impact

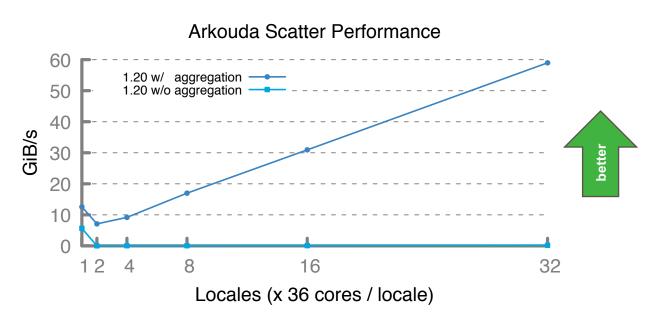


- Significant performance improvements for operations with fine-grained comm
 - Following results are from:
 - 32-node Cray CS with 56 Gb InfiniBand network
 - 512-node Cray XC with Aries network
 - Per-node hardware is similar for both systems
 - 36-core Broadwell CPU
 - 128 GB RAM

Arkouda Aggregation: Cray CS Impact



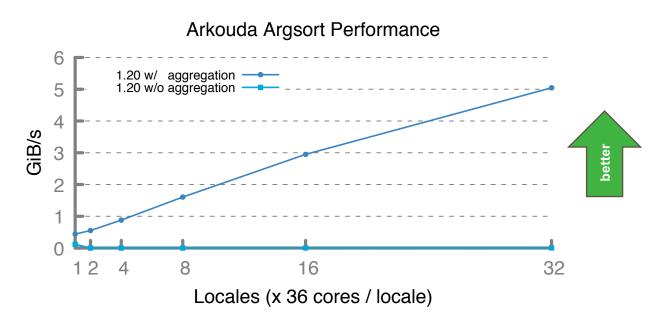
- Significant performance improvements for operations with fine-grained comm
 - 300x speedup for scatters on 32 CS nodes



Arkouda Aggregation: Cray CS Impact



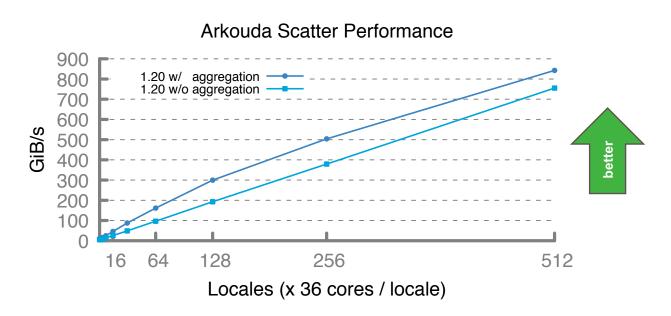
- Significant performance improvements for operations with fine-grained comm
 - 1200x speedup for sorting on 32 CS nodes



Arkouda Aggregation: Cray XC Impact



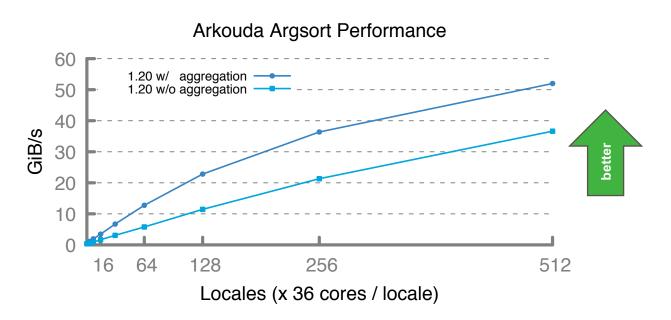
- Significant performance improvements for operations with fine-grained comm
 - 10% speedup for scatters on 512 XC nodes



Arkouda Aggregation: Cray XC Impact



- Significant performance improvements for operations with fine-grained comm
 - 40% speedup for sorting on 512 XC nodes



Arkouda Aggregation: Next Steps



- Optimize aggregation performance and reduce memory footprint
 - Current implementation is simple, lots of optimization opportunity
- Improve aggregation ease-of-use
 - Add utility functions for common idioms (gather/scatter)
 - Possibly enable with automatic unordered compiler optimization
- Add aggregation to Chapel's standard library

Arkouda Chapel Performance: This Effort

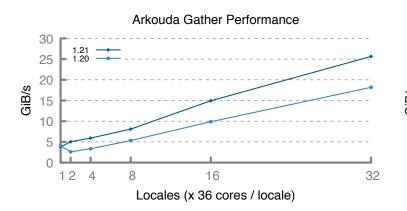


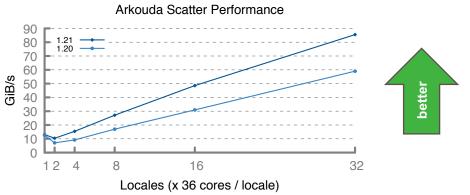
- Many 1.21 optimizations were motivated by, and benefitted, Arkouda
 - Optimizing on-statements for InfiniBand networks benefitted aggregation
 - Optimizing distributed array/domain creation benefitted most operations
 - Extending fast-followers improved array binary operations

Arkouda Chapel Performance: Cray CS Impact



- Significant performance improvements on Cray CS (FDR InfiniBand)
 - At 32 locales: 40% faster Gather, 45% faster Scatter

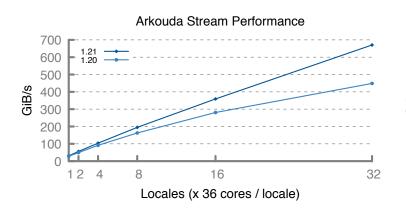


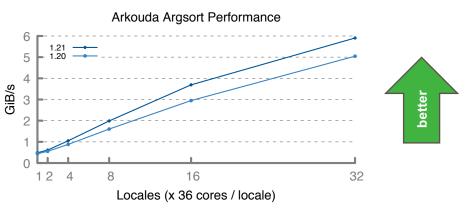


Arkouda Chapel Performance: Cray CS Impact



- Significant performance improvements on Cray CS (FDR InfiniBand)
 - At 32 locales: 50% faster Stream, 15% faster Argsort

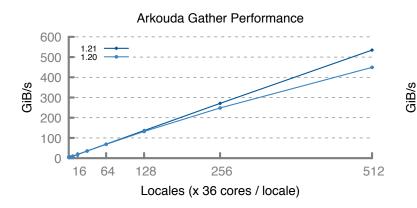




Arkouda Chapel Performance: Cray XC Impact



- Significant performance improvements on Cray XC (Aries)
 - At 512 locales: 20% faster Gather, 5% faster Scatter

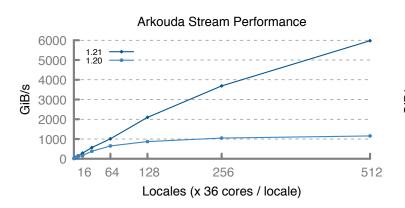


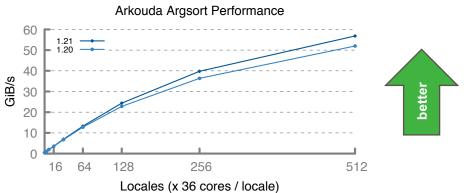


Arkouda Chapel Performance: Cray XC Impact



- Significant performance improvements on Cray XC (Aries)
 - At 512 locales: 525% faster Stream, 10% faster Argsort





Arkouda: Additional Performance Improvements

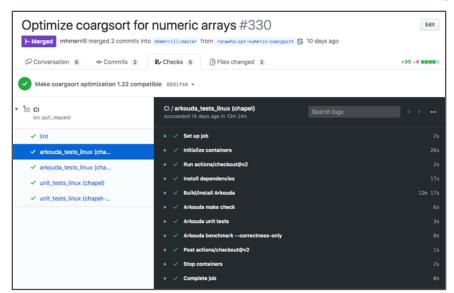


- A few other Arkouda-specific optimizations were contributed upstream
 - Eliminated overhead for sorting negative integers
 - Optimized hashing used for string sorting
 - Requires extremely fast serial performance and scalable operations
 - Showcases Chapel's ability to program in the small and large

Arkouda: CI Testing



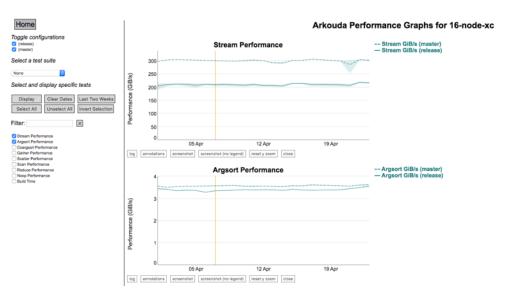
- Added continuous integration (CI) testing
 - Build and test Arkouda for each Pull Request



Arkouda: Performance testing



- Added benchmarking infrastructure and nightly performance testing
 - Runs single-node, 16-node CS, and 16-node XC
 - https://chapel-lang.org/perf/arkouda/

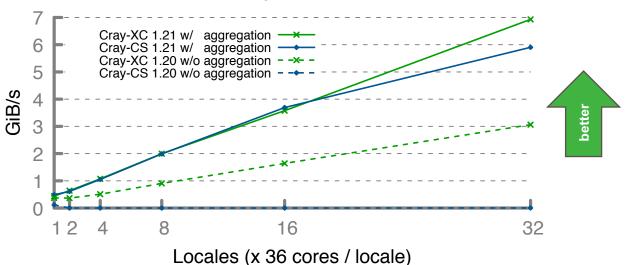


Arkouda: Summary



- Arkouda performance has significantly improved
 - Particularly on InfiniBand, which is now comparable to Aries

Arkouda Argsort Performance



User Applications: Next Steps



- Continue to support user efforts
 - Please feel free to contact us if your Chapel code needs tuning
- Develop better tooling for profiling and performance investigation
- Improve tooling for building/testing/releasing Chapel packages and applications
 - i.e. improve Mason

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