Scalable Tools for Analysis of Massive Remote-Sensing Datasets on High-Performance Computers

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Introduction

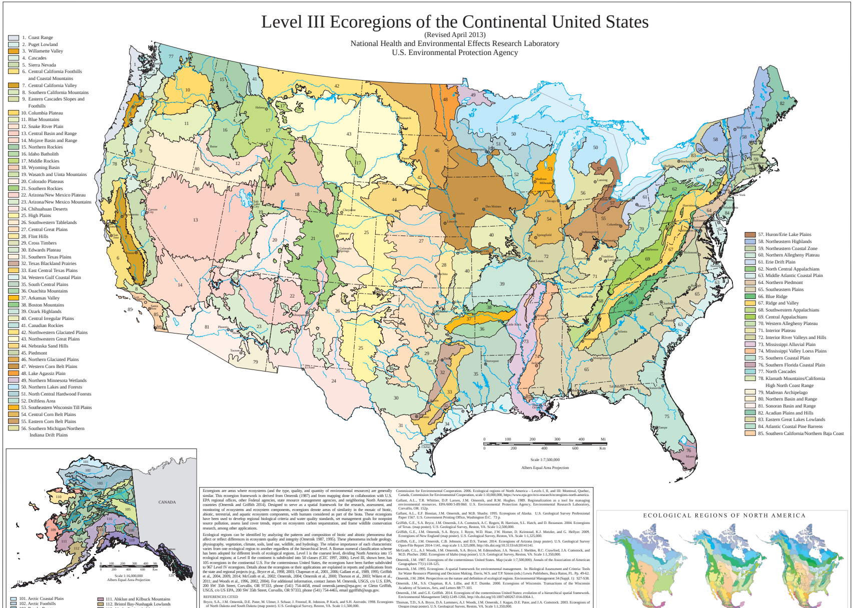
- Increasing availability of high-resolution geospatiotemporal data sets from varied sources:
  - Observatory networks
  - Remote sensing platforms
  - Computational Earth system models
- New possibilities for knowledge discovery and mining of geoscience data sets fused from disparate sources.
- Traditional tools impractical for analysis/synthesis of data sets this large: Need new approaches to utilize complex memory hierarchies and high levels of available parallelism in state-of-the-art high-performance computing platforms.
- We have adapted pKluster—an open-source tool for accelerated *k*-means clustering we use for many geospatiotemporal applications—to effectively utilize state-of-the art multi- and manycore processors, such as the second-generation Intel Xeon Phi ("Knights Landing") processor, as well as GPGPUs.

Scalable *k*-means Clustering with pKluster

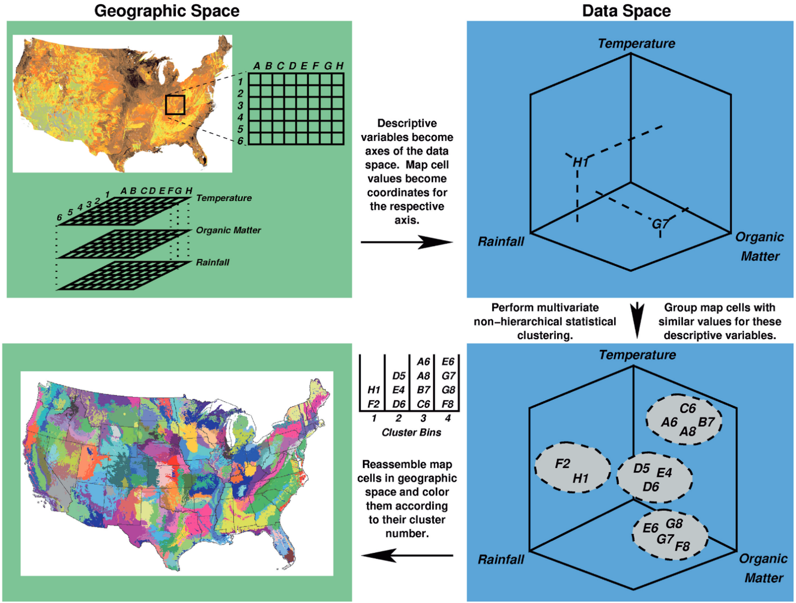
Our distributed-memory clustering code has a long history...

Figure: Originally developed in 1996–1997 for use on the Stone Soupercomputer, a very early Beowulf-style cluster constructed entirely out of surplus parts (see "The Do-It-Yourself Supercomputer", *Scientific American*, 265 (2), pp. 72-79, 2001.)

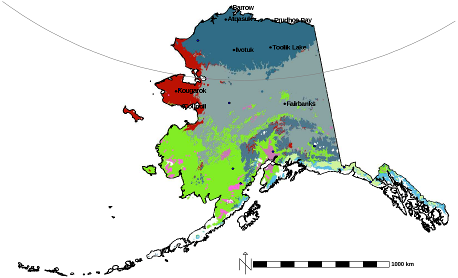
Original motivation: Replacing hand-drawn ecoregionalizations



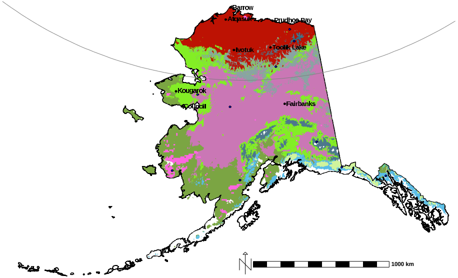
Quantitative Ecoregionalization through Multivariate Spatio(-Temporal) Clustering



Quantitative Ecoregionalization through Time: Sampling Network Design



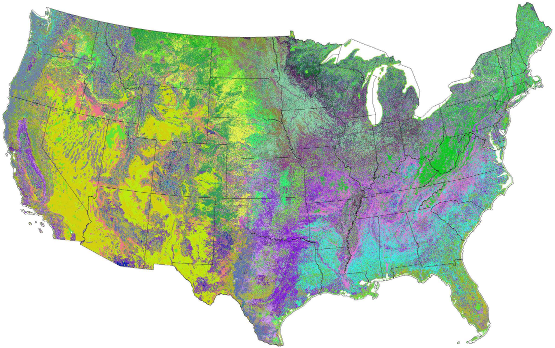
(a) 10 ecoregions, present (2000-2009)

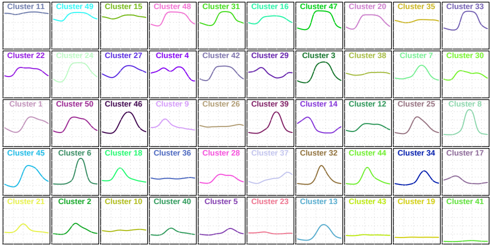


(b) 10 ecoregions, future (2090-2099)

Figure: Geospatiotemporal clustering of a combination of observational data and downscaled general circulation model results projects dramatic shifts in location of Alaska ecoregions using downscaled 4 km GCM results. Arctic tundra projected to be at 0.78% of current extent by 2099. DOI: 10.1007/s10980-013-9902-0.
2014 US-IALE Outstanding Paper in Landscape Ecology.

MODIS NVDI-based phenoregionalization





GSMNP LiDAR-derived canopy structure classification

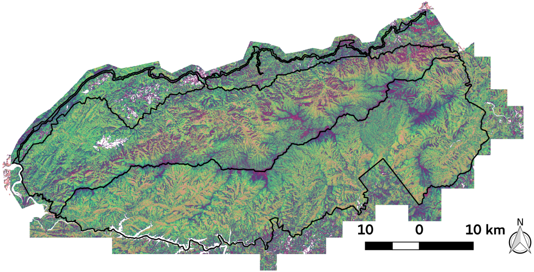
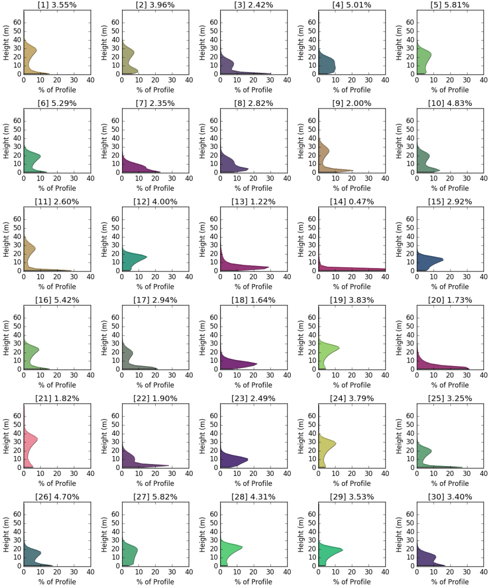


Figure: Map (above) showing the 30 most-different classes of vegetation canopy structure, as identified by k-means clustering (right) for the Great Smoky Mountains National Park.



Scalable *k*-means Clustering with pKluster: Parallel Computers Have Evolved!

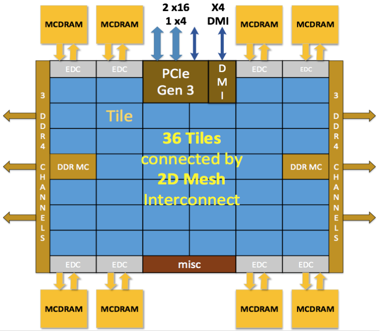
- When pKluster was initially written, on-node parallelism was virtually nonexistent on commodity PCs; focus was purely on distributed-memory parallelism (i.e., Message Passing Interface—MPI).
- Modern HPC compute nodes increasingly feature high degrees of on-node parallelism:
  - Modern CPUs feature large numbers of compute cores, increasing reliance on SIMD (vector instructions).
  - Many new supercomputers are concentrating almost all power in GPU "accelerators".

Figure: O. G.

Figure: New School

Manycore Computing Architectures

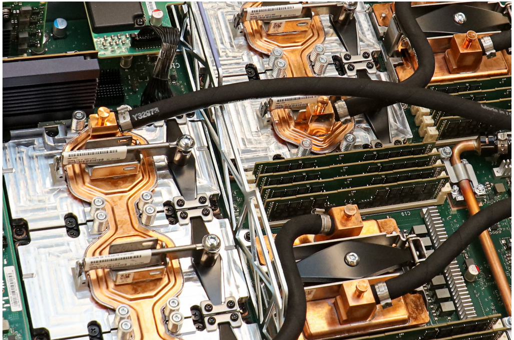
- In recent years, the number of compute cores and hardware threads has been dramatically increasing.
- Seen in GPGPUS, “manycore” processors such as the Intel Xeon Phi, and even on standard server processors (e.g., Intel Xeon Skylake).
- There is also increasing reliance on data parallelism/fine-grained parallelism.
  - Current Intel consumer-grade processors have 256-bit vector registers and support AVX2 instructions.
  - Second-generation Intel Xeon Phi processors and Intel Xeon (Skylake and beyond) server processors have 512-bit vectors/AVX512 instructions.



At left, “Knights Landing” (KNL) Xeon Phi processor:

- Up to 36 tiles interconnected via 2D mesh
- Tile: 2 cores + 2 VPU/core + 1 MB L2 cache
- Core: Silvermont-based, 4 threads per core, out-of-order execution
- Dual issue; can saturate both VPUs from a single thread
- 512 bit (16 `floats` wide) SIMD lanes, AVX512 vector instructions
- High bandwidth memory (MCDRAM) on package: 490+ GB/s bandwidth on STREAM triad[2]
- Powers the NERSC Cori and ALCF Theta supercomputers

OLCF Summit Supercomputer



System totals

- $\sim$ 200 PFlop/s theoretical peak
  143 PFlop/s LINPACK—#1 in TOP500
- 4,608 compute nodes

Node configuration

- Compute:
  - Two IBM Power9 CPUs, each 22 with cores, 0.5 DP TFlop/s
  - Six NVIDIA Volta V100 GPUs, each with 80 SMs–32 FP64 cores/SM, 7.8 DP TFlop/s
- Memory:
  - 512 GB DDR4 memory
  - 96 (6×16) GB high-bandwidth GPU memory
  - 1.6 TB nonvolatile RAM (I/O burst buffer)

Almost all compute power is in GPUs!

CPU Benchmarking Platforms and Problem

Performance benchmarking platforms:

	Intel Xeon E5-2697 v4	Intel Xeon Gold 6148	Intel Xeon Phi 7250
Code Name	Broadwell (BDW)	Skylake (SKX)	Knights Landing (KNL)
Sockets	2	2	1
Cores	36	40	68
Threads	72	80	272
CPU clock	2.3 GHz	2.4 GHz	1.4 GHz
High-bandwidth memory	-	-	16 GB
DRAM	128 GB @ 2400 MHz	192 GB @ 2666 MHz	98 GB @ 2400 MHz
Instruction set architecture	AVX2	AVX-512F,DQ,CD,BW,VL	AVX-512F,PF,ER,CD
Theoretical peak flops (FP32 / FP64)	2649 / 1324	6144 / 3072	6092 / 3046

- SKX and KNL double the SIMD width of BDW (256 to 512 bits)
- SKX and KNL have similiar peak flops; KNL more dependent on SIMD and thread parallelism

Benchmark problem: GSMNP LiDAR clustering

- 1.5 million observations
- 74 dimensions
- $k = 2000$ clusters

Parallel k-means clustering algorithm

k-means clustering

Goal: Partition data into k clusters, such that centroid c_j minimizes the total distance $D_j = \sum d(c_j, a)$ to points a in cluster P_j.
Iterative calculation: Given initial partition, find centroid of each cluster and repartition according to closest centroid (essentially Lloyd's algorithm, or voronoi relaxation).

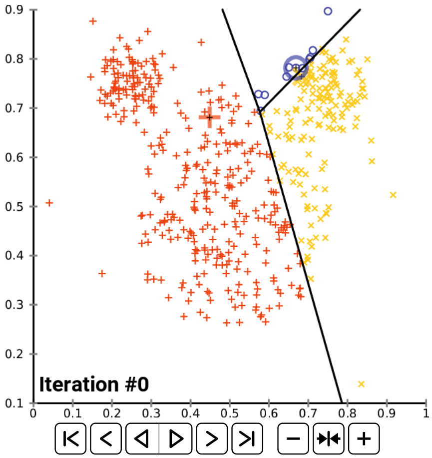


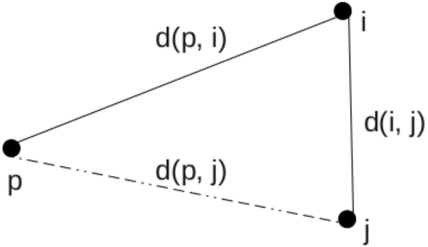
Figure: Illustration of k-means iteration for $k = 3$. https://commons.wikimedia.org/wiki/File:K-means_convergence.gif

Parallel implementation in *pKluster*

- Centralized master-worker paradigm
- Start from some initial centroids (chosen offline)
- Master:
  - Broadcasts centroids and aliquot assignment to workers
  - Collects new cluster assignments from workers
  - Recomputes centroids
- Workers, for an assigned aliquot:
  - Compute observation-to-centroid distances
  - Assign each observation to closest centroid

Accelerated k-means clustering

- Classical k-means actually performs far more distance calculations than required!
- Use the triangle inequality to eliminate unnecessary point-to-centroid distance computations based on the previous cluster assignments and the new inter-centroid distances.
- Reduce evaluation overhead by sorting inter-centroid distances so that new candidate centroids c_j are evaluated in order of their distance from the former centroid c_i. Once the critical distance $2d(p, c_i)$ is surpassed, no additional evaluations are needed, as the nearest centroid is known from a previous evaluation.



$d(i,j) \leq d(p,i) + d(p,j)$
$d(i,j) - d(p,i) \leq d(p,j)$
if $d(i,j) \geq 2d(p,i)$:
$\quad d(p,j) \geq d(p,i)$
$\quad$ without calculating the distance $d(p,j)$

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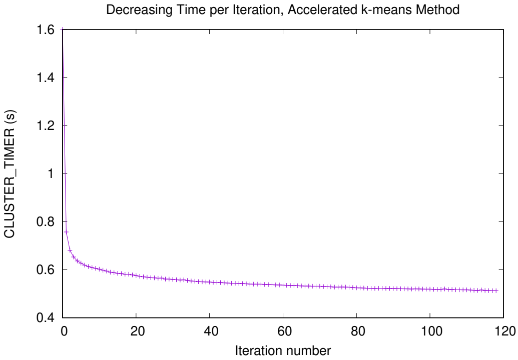
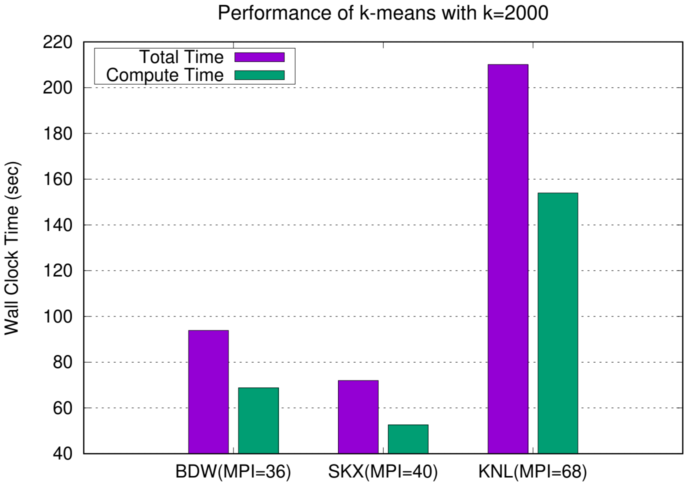


Baseline (accelerated *k*-means) Performance

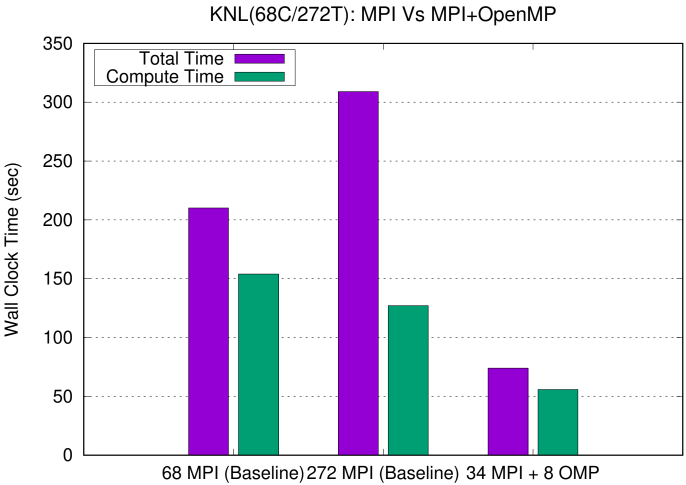


- 1.3X speedup on SKX vs. BDW
- Significant slowdown (2.2X) on KNL vs. BDW

Effective Use of Hyperthreads

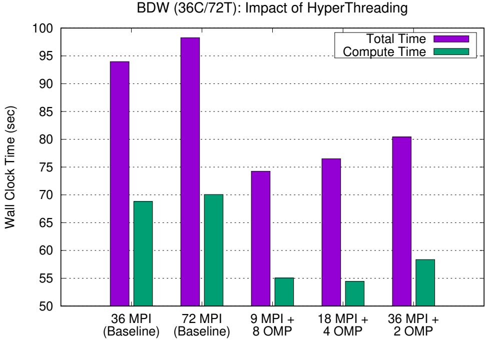
- Using a pure MPI approach (one MPI rank per core), performance of the accelerated k-means clustering approach is surprisingly poor on the "Knights Landing" (KNL) processor.
- Using two MPI ranks per core slightly decreases time in the actual clustering calculation, but slightly increases total time due to greater overhead in master-worker coordination.
- This suggests that using more available hardware threads can improve performance on KNL, if we can avoid increasing master-worker overhead.

Performance Optimizations: OpenMP Parallelism on KNL

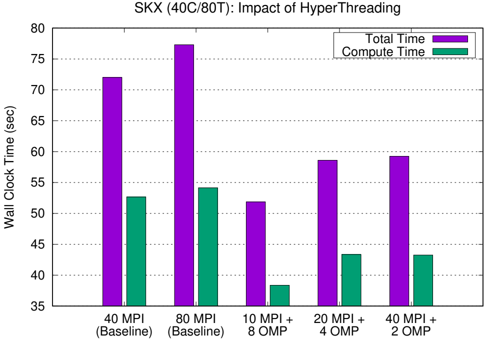


- Hybrid MPI-OpenMP version of distance calculation function effectively utilizes FMA units and reduces the bottleneck on rank 0.
- Use dynamic loop scheduling to smooth load imbalance due to triangle inequality (many observations in an aliquot might skip point-to-centroid distance calculation).
- Pin each MPI to a KNL "tile" and spawn 8 threads (4 threads per core).
- 2.8X improvement.

Performance Optimizations: OpenMP Parallelism on BDW and SKX



(a) Intel Xeon E5-2697 v4 ("Broadwell")



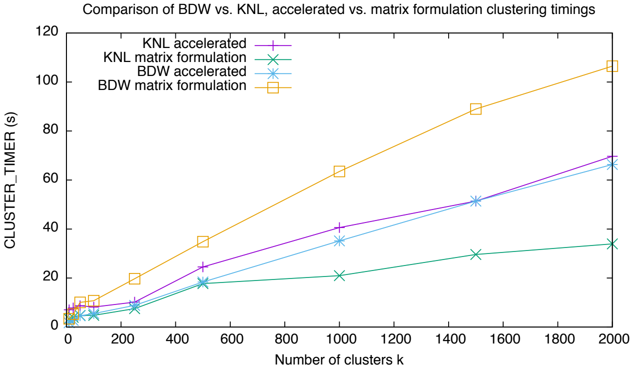
(b) Intel Xeon Gold 6148 ("Skylake")

Figure: Comparison of times to cluster the GSMNP LiDAR data set with $k = 2000$ on the Broadwell (BDW) and Skylake (SKX) Xeon processors for different numbers of MPI ranks and OpenMP threads.

Improving computational intensity

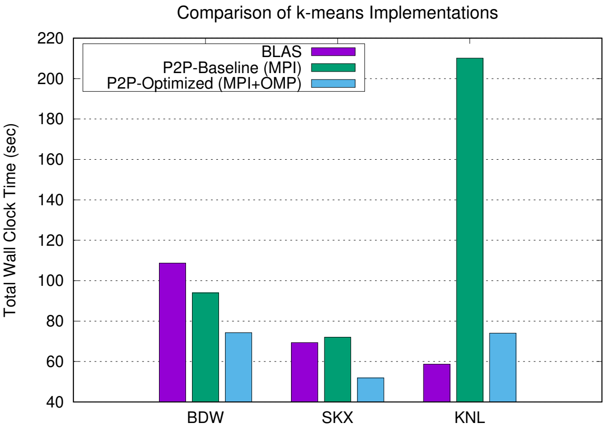
- Can achieve greater computational intensity of the observation–centroid distance calculations by expressing the calculation in matrix form:
  - For observation vector x_i and centroid vector z_j, the squared distance between them is $D_{ij} = \left\|x_i - z_j\right\|^2$.
  - Via binomial expansion, $D_{ij} = \|x_i\|^2 + \left\|z_j\right\|^2 - 2x_i \cdot z_j$.
  - The matrix of squared distances can thus be expressed as $D = \overline{x}\mathbf{1}^\intercal + \mathbf{1}\overline{z}^\intercal - 2X^\intercal Z$, where X and Z are matrices of observations and centroids, respectively, stored in columns, $\overline{x}$ and $\overline{z}$ are vectors of the sum of squares of the columns of X and Z, and $\mathbf{1}$ is a vector of all 1s.
- Above expression can be calculated in terms of a level-3 BLAS operation (xGEMM), followed by two rank-one updates (xGER, a level-2 operation).
- We use highly optimized BLAS implementations from Intel's MKL and NVIDIA cuBLAS to speed up distance calculations on Xeon Phi and GPGPUs, respectively.
- Distance calculations using above formulation can be dramatically faster than the straightforward loop over vector distance calculations when many distance comparisons must be made.
- Using the matrix formulation for distance comparisons in early k-means iterations is straightforward; a more complicated approach we hope to explore is using the matrix formulation in combination with the acceleration techniques described above, in which only a subset of observation–centroid distances are calculated.

BDW vs. KNL, Accelerated (MPI + OpenMP version) vs. Matrix Formulation



- Though BLAS/matrix formulation performs many more distance calculations, xGEMM is so efficient on KNL that it outperforms acceleration scheme for all k; also shows slowest growth in cost as k increases.
- On BDW, matrix formulation only benefits initial iterations (when many distance comparisons are required); after that, acceleration technique results in dramatically faster iterations.

Performance Improvements Summary

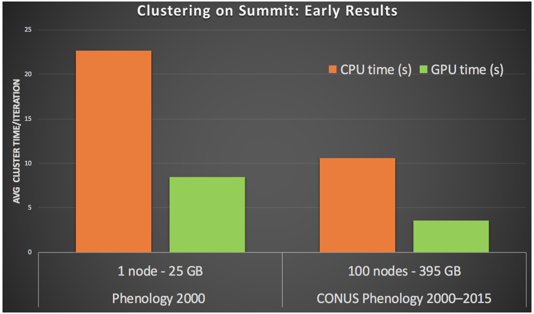


- BLAS formulation yields best performance on KNL, despite many more distance calculations than point-to-point (P2P) approach using "acceleration"; slightly slower then P2P distance calculation on SKX.
- Best performance on SKX with acceleration, though difference between matrix and accelerated algorithm is smaller—consistent with the improved xGEMM performance on SKX compared to BDW
- Overall performance improvements:
  - KNL: 3.5X
  - BDW: 1.3X
  - SKX: 1.4X

Early Summit Benchmarking Results

The matrix formulation for the distance calculations facilitates using GPUs on Summit: Replace BLAS calls with NVIDIA cuBLAS calls.

Problem Config	Data Size	# Clusters	Nodes	CPU time/iter	GPU time/iter	Speedup
Phenology 2000	25 GB	1000	1	22.69 s	8.47 s	2.67
Phenology 2000–2015	395 GB	1000	100	10.60 s	3.59 s	2.95



Future Directions

pKluster software development

- Investigate hybrid approach combining accelerated k-means method and matrix formulation within the same iteration.
- Re-implement a fully distributed, masterless approach in the current version of the code to handle cases in which master-slave overhead is high (e.g., many cases on `KNL`).
- Add support for emerging high-capacity, non-volatile memory technologies.
- Supported open-source release under Apache License 2.0.
- Explore integration with Portable, Extensible Toolkit for Scientific Computation (PETSc), or reimplementation of our algorithms in PETSc.

Complementary machine-learning techniques

- Sophisticated neural networks becoming more accessible
  - High level frameworks like Keras allow easy utilization of libraries such as TensorFlow
  - Consumer-grade GPUs are enabling expensive training even without access to expensive HPC hardware
- Open-source PETSc-based support vector machine (SVM) implementations allow scalable training of SVMs