

# Parallel $k$ -Means Clustering for Quantitative Ecoregion Delineation Using Large Data Sets

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# Outline

- **Introduction:** Delineation of ecoregions
- **Computational challenges:** Spatio-temporal scales of data and data set size
- **Design:** Parallel  $k$ -means algorithm and enhancements
- **Performance:** Parallel performance and scaling
- **Application:** Forest threat detection using MODIS NDVI products

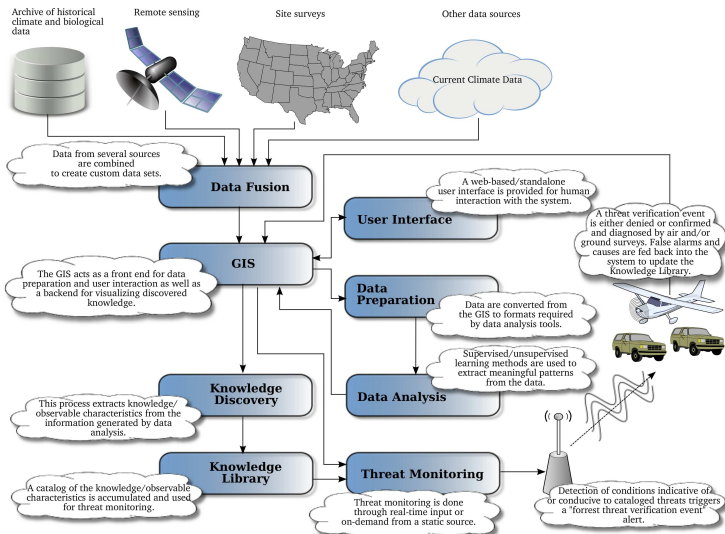


# Introduction

- **Ecoregions** are geographical regions of generally similar combination of ecologically relevant conditions like temperature, precipitation and soil characteristics.
- Understanding and delineation of ecoregions are useful for predicting suitable species range, stratification of ecological samples, and to help prioritize habitat preservation and remediation efforts.
- In the case of threatened or endangered species, a well-executed ecoregion classification can be used to identify and locate the extent of suitable habitat for the purposes of preserving or improving it.
- Large amount of data sets are available from satellite, airborne and ground based remote sensing; GCM model outputs
- Data mining tools can be used to extract knowledge from these data sets



# Overview of the Forest Incident Recognition and State Tracking (FIRST) System





## Normalized Difference Vegetation Index (NDVI)

- NDVI exploits the strong differences in plant reflectance between red and near-infrared wavelengths to provide a measure of “greenness” from remote sensing measurements.

$$\text{NDVI} = \frac{(\sigma_{\text{nir}} - \sigma_{\text{red}})}{(\sigma_{\text{nir}} + \sigma_{\text{red}})} \quad (1)$$

- These spectral reflectances are ratios of reflected over incoming radiation,  $\sigma = I_r/I_i$ , hence they take on values between 0.0 and 1.0. As a result, NDVI varies between  $-1.0$  and  $+1.0$ .
- Dense vegetation cover is 0.3–0.8, soils are about 0.1–0.2, surface water is near 0.0, and clouds and snow are negative.

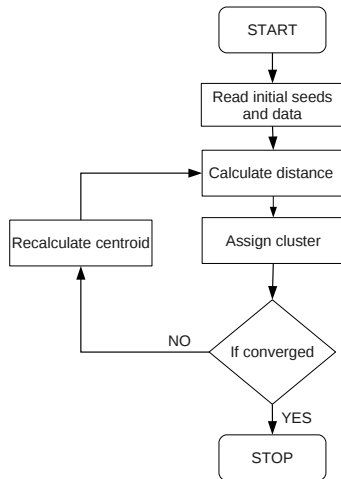


## Data Mining for Change Detection

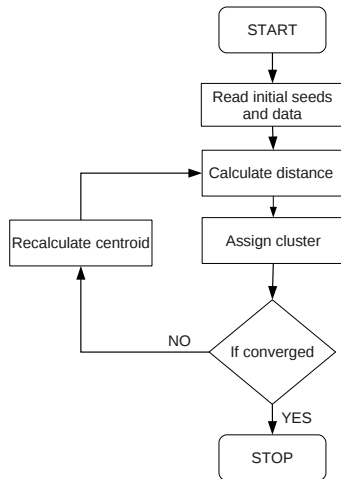
- Changes in forest states are captured by the remote sensing.
- Difficult to use map arithmetic, since the appropriate choice of parameters may vary by region and/or type of forest disturbance.
- An automated, unsupervised change detection system is desired.
- We apply geospatiotemporal data mining techniques to perform unsupervised classification
- Further analysis of clustering outputs for change detection
- Identify unexpected changes in forest states.



# *k*-means cluster algorithm



## $k$ -means cluster algorithm



- Serial algorithm
- Requires enough memory to hold all the data
- Not adequate for the large data sets of our interest

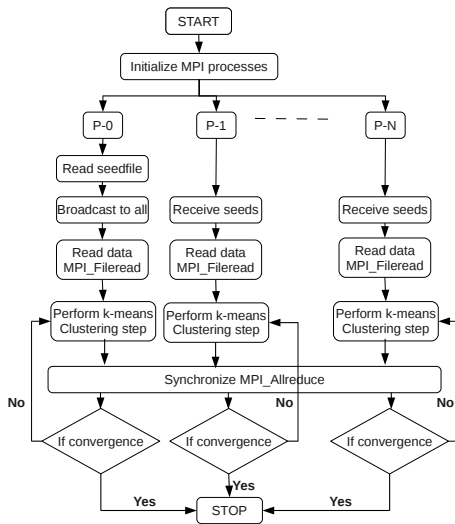


## Clustering the MODIS NDVI data

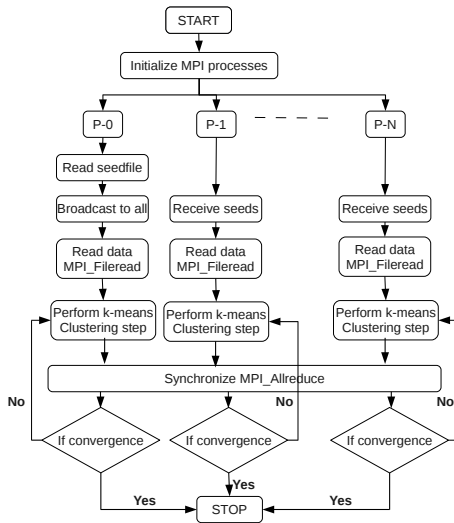
- Data from MODIS: Continental US at 250m resolutions, 16 days
- The ~22B NDVI values in the data set are arranged as annual NDVI traces of 22 values, for each grid cell (~146.4M records) in each of the seven yearly maps (2003-2009),
- The entire set of NDVI traces for all years and map cells is combined into one 84 GB (single precision binary) data set of 22-dimensional “observation” vectors that are analyzed via the  $k$ -means algorithm.
- After applying  $k$ -means, cluster assignments are mapped back to the map cell and year from which each observation came, yielding seven maps in which each cell is classified into one of  $k$  phenoclasses
- The phenoclasses form a “dictionary” of representative or prototype annual NDVI traces (the cluster centroids) derived from the full spatiotemporal extent of the observations in the input



# Parallel $k$ -means cluster algorithm



## Parallel $k$ -means cluster algorithm

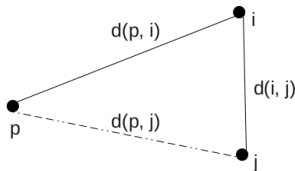


- Masterless parallel algorithm
- Data partitioned across distributed memory processors
- Triangular inequality based acceleration
- Warping to handle any null clusters
- Suitable for very large data sets



## Enhancements to $k$ -means algorithm

Triangular inequality based  
acceleration (Phillips 2002):



$$d(i, j) \leq d(p, i) + d(p, j)$$

$$d(i, j) - d(p, i) \leq d(p, j)$$

if  $d(i, j) \geq 2d(p, i)$  :

$$d(p, j) \geq d(p, i)$$

without calculating the distance

$d(p, j)$

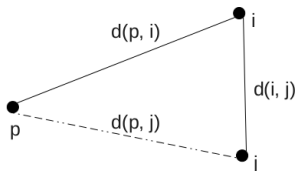
- Calculate inter-centroidal distances
- Sort the inter-centroidal distances





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- Calculate inter-centroidal distances
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### Warping to handle null clusters:

- Avoid empty clusters
- Move “worst of the worst” point to the empty cluster
- Update cluster sizes and recalculate centroid

Phillips, S. J. (2002) “Acceleration of K-Means and Related Clustering Algorithms”, ALENEX '02: Revised Papers from the 4th International Workshop on Algorithm Engineering and Experiments, Springer-Verlag, 2002, 166-177



## Data sets and resources used

### Summary of data sets used

Dataset	No. of dimensions	No. of records	Dataset size
fullUS	25	7,801,710	745 MB
AmeriFlux	30	7,856,224	900 MB
Phenology	22	1,024,767,667	84 GB



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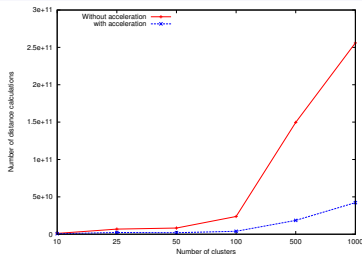
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### Jaguar Cray XT5 (ORNL):

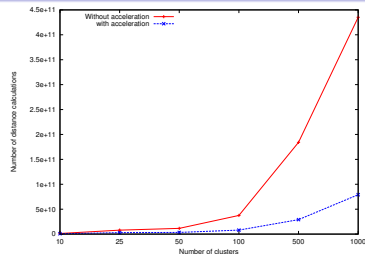
- 18,688 compute nodes
  - Dual hex-core AMD Opteron 2435 (istanbul) processors  
2.6GHz
  - 16GB DDR2-800 memory
- Seastar 2+ router
- Parallel lustre filesystem
- Peak performance: 2.3 petaflops/s



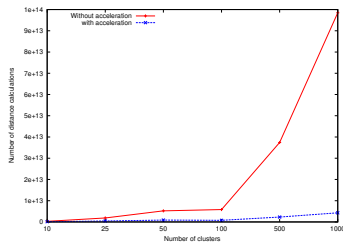
# Effect of acceleration: Scaling with increasing $k$ and $n$ : No. of distance calculations



fullUS data set



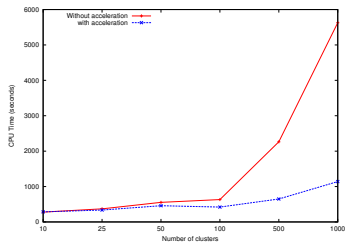
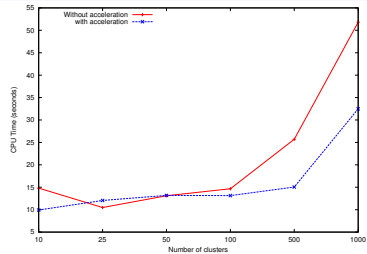
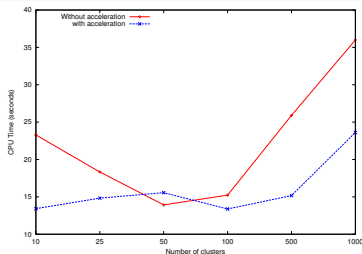
Ameriflux data set



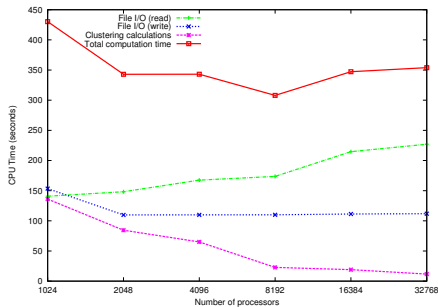
Phenology data set



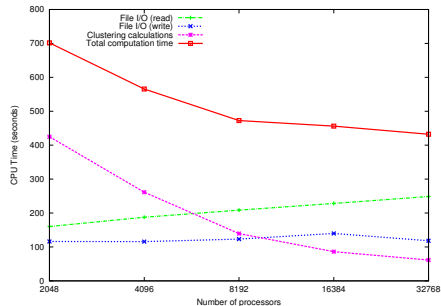
# Effect of acceleration: Scaling with increasing $k$ and $n$ : CPU time



## Strong scaling test: Phenology data set



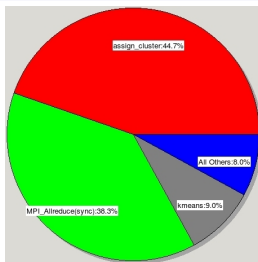
No. of clusters ( $k$ ) = 50



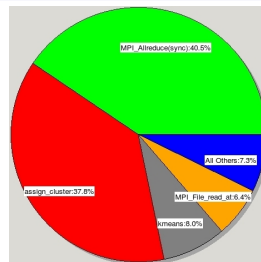
No. of clusters ( $k$ ) = 1000



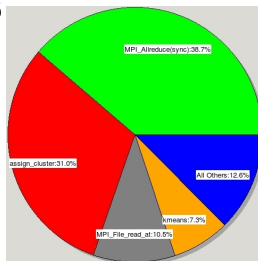
# CrayPat summary: Phenology data set, 1000 clusters



Num. procs = 256



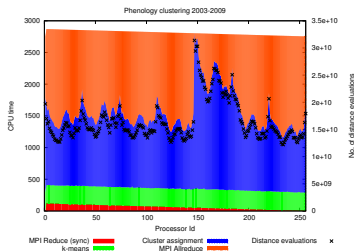
Num. procs = 512



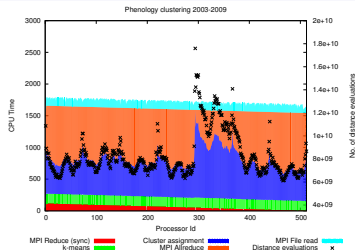
Num. procs = 1024



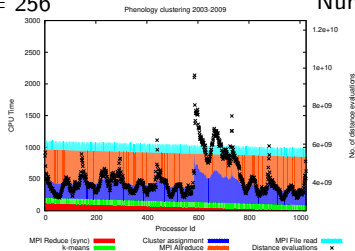
# Performance results: Phenology data set, 1000 clusters



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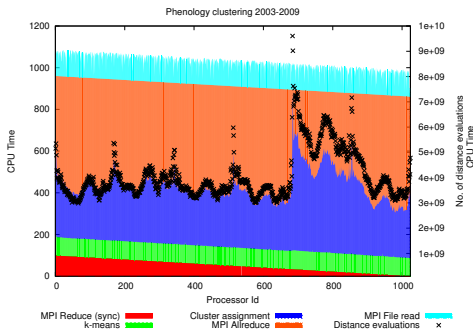


Num. procs = 1024

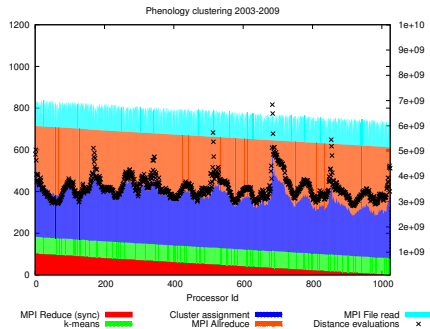




# Performance results: Phenology data set, 1000 clusters, 1024 procs



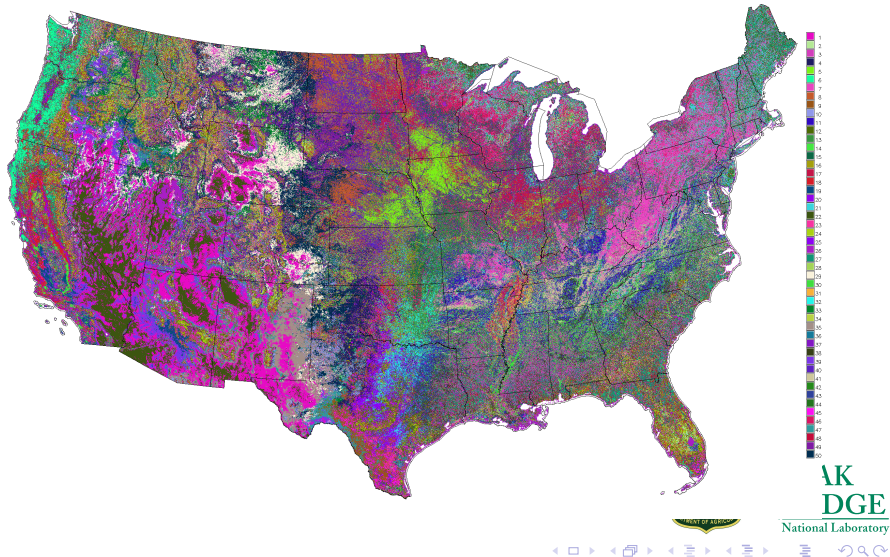
Phenology 2003-2008



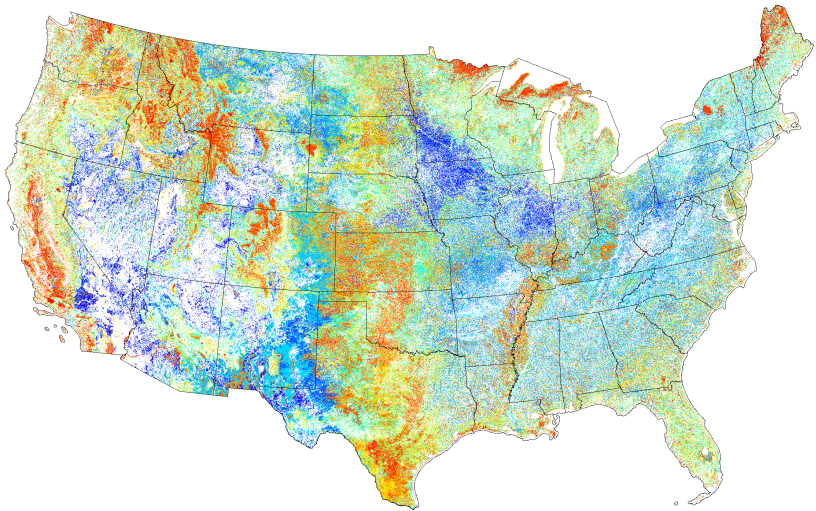
Phenology 2003-2009 (without 2007)



## 50 Phenoregions for Year 2009 (Clustering 2003-2009)

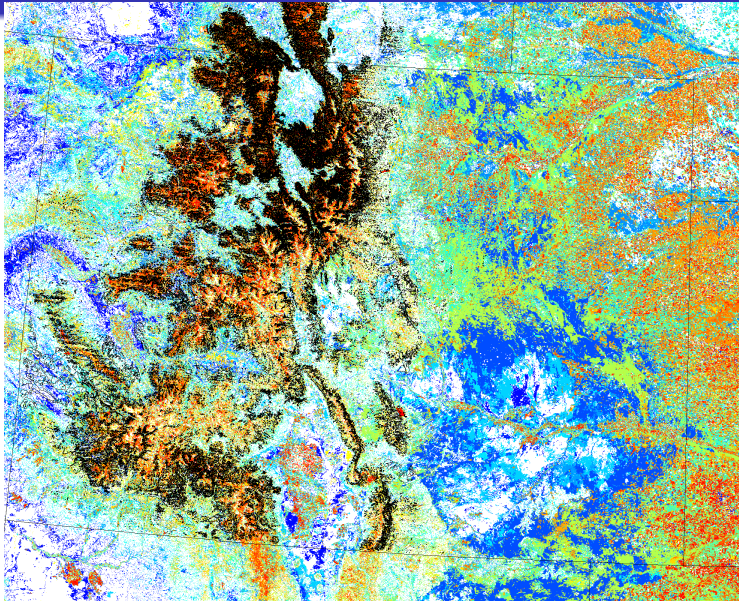


## Transition distance map (2003-2008)



AK  
RIDGE  
National Laboratory

## Mountain Pine Beetle in Colorado for (2008 – 2003)



# Conclusions

- Parallel  $k$ -means cluster analysis tool enables the analysis of very large earth sciences data sets
- Enhancements for improved performance of the algorithm
- Scalable design for large data sets
- Good parallel performance and scaling achieved on state-of-the-art supercomputers
- Promising results for geospatiotemporal cluster analysis of phenology from MODIS NDVI
- Successfully applied for forest threat detection; global climate model data comparison (CMIP)



## Future Work

- Two-phase I/O for improved parallel I/O performance
- Improved load balancing: block cyclic distribution of data, dynamic load balance
- Support for fuzzy and hierarchical clustering
- Cluster analysis of updated NDVI data sets: 2000-2010(part), every 8 days (200 GB data)
- Cluster analysis for comparison of global climate model results for CMIP5



# Acknowledgments

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# Thank you!

## Questions?

Mills, Hoffman, Kumar and Hargrove: “Cluster Analysis-Based Approaches for Geospatiotemporal Data Mining of Massive Data Sets for Identification of Forest Threats”, Session 21b, 2:30PM



Image source: <http://blogs.denverpost.com/thespot/files/2010/02/barkbeetle.jpg>